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Julia Schuster

Random Graph Models and their Application to Biological Networks

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Random Graph Models and their Application to Biological Networks

Autorin:
Julia Schuster

Studiengang:
Diskrete und Computerorientierte Mathematik

Seminargruppe:
ZD10w1

Erstprüfer:
Prof. Dr. Klaus Dohmen

Zweitprüfer:
Prof. Dr. Peter Tittmann

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Referat

Diese Masterarbeit beschäftigt sich mit verschiedenen Modellen von Zufallsgraphen für biologische Netzwerke. Nach einer kurzen Einführung, in der benötigte graphentheoretische Begriffe sowie Anwendungsbeispiele der Graphentheorie erläutert werden, erfolgt die Vorstellung von drei einfachen Zufallsgraphenmodellen: das *Erdős-Rényi-Modell*, das *Gilbert-Modell* und das p_1*-Modell*. Außerdem werden in diesem Kapitel zwei spezielle Zufallsgraphenmodelle, zum einen die *Exponential Random Graph Models* und zum anderen die *Small-World Models*, ausführlich dargestellt. Anschließend werden alle Modelle für ein konkretes biologisches Netzwerk, das Protein-Protein-Interaktions-Netzwerk des Bakteriums Escherichia coli, auf ihre Anwendbarkeit überprüft und diesbezüglich bewertet.

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V. List of Symbols

$\mathbb{N}$	Set of natural numbers without zero, i.e. $\mathbb{N} = \{1,2,3,...\}$
$\mathbb{N}_0$	Set of natural numbers including zero, i.e. $\mathbb{N}_0 = \{0,1,2,3,...\}$
$\mathbb{R}$	Set of real numbers
$\mathbb{R}_{\geq 0}$	Set of real numbers greater or equal to zero
G, H	Network or graph
V	Set of vertices with $\|V\| = n$ being the number of vertices
E	Set of edges with $\|E\| = m$ being the number of edges
$A = (a_{ij})_{n,n}$	Adjacency matrix of a graph
d_i	Degree of a vertex i in an undirected graph
$d_i^{(in)}, d_i^{(out)}$	In- and out-degree of a vertex i in a directed graph
QM	Quality measure
ERGM	Exponential Random Graph Models
E. coli	Bacterium Escherichia coli
PPIN	Protein-protein interaction networks

1 Introduction

Nowadays modelling networks is an important field of mathematics for many reasons. The first one is that with models complex networks can be simplified and so the network is easier to understand and coherences of certain structures can be found. Another advantage of modelling is the simulation of networks with few parameters. From these simulations hypotheses can be made and proved and also generalizations of a network are possible, so that the model can explain the impact of some structures on the network. [20]
On that account, this master thesis studies various graph models and their application to biological networks. Especially random graph models are examined and several random graph models are presented in Chapter 2. Afterwards, Chapter 3 will test the fitting of the described models to a sample biological network.
At first a brief overview of required terms of graph theory is given and some examples of networks are illustrated.

1.1 Graph Theory

This section will give a short introduction into graph theory for a better understanding of the following chapters. Therefore some basic definitions and formulas are given.

Definition 1.1: A *network* or *graph* is a pair $G = (V, E)$, where V is the set of *vertices* or *nodes* and E is the set of *edges* between these vertices such that E contains 2-element subsets of V.
A *sub-network* or *sub-graph* of G is a graph $H = (W, F)$ with $W \subseteq V$ and $F \subseteq E$.

The number of vertices of G is given by $n = |V|$ and the number of edges is $m = |E|$. An edge $e \in E$ between two vertices $i, j \in V$ can be directed, which is written as $e = (i, j)$, or undirected and is then written as $e = \{i, j\}$. If all edges are directed the graph is called *directed graph* and all edges are ordered pairs of vertices, which means $E \subseteq V^2$ and there are at most n^2 different edges. If all edges are undirected the graph is called *undirected graph* and the edges are unordered pairs of vertices, so it is $E \subseteq [V]^2$ and $m \leq \binom{n}{2} + n$. Two vertices i, j, which are connected by an edge e are called *adjacent* and e is *incident* to node i and j. All vertices, which are adjacent to a vertex i, are called *neighbours* of i. The information which vertices are connected can be represented by the *adjacency matrix* $A = (a_{ij})_{n,n}$ where a_{ij} is the number of edges between vertex i and vertex j. For undirected graphs the adjacency matrix is symmetric, but for directed graphs this may not be the case.
A special edge is the *self loop* where the edge connects a vertex with itself, i.e. $e = (i, i)$ and $e = \{i, i\}$, respectively. If two vertices i, j are connected by more than one edge,

these edges are called *multiple edges*. A graph without self loops and multiple edges is named *simple graph* and its adjacency matrix is a binary matrix with $a_{ii} = 0, \forall i \in V$. If there are two contrary directed edges e_1, e_2 between two vertices i, j, that is, it exists $e_1 = (i, j)$ and $e_2 = (j, i)$, then e_1 and e_2 are called *reciprocated* or *anti-parallel*.
Two special graphs are the *edgeless graph*, which has no edges at all and so its edge set is $E = \emptyset$, and the *complete graph*, where all possible edges exists, in other words $E = V^2$ and $E = [V]^2$, respectively.

Some important terms of graph theory for undirected graphs and their explanations are given in Table 1.1.

Table 1.1: Some terms of graph theory for undirected graphs

term	**explanation**
(vertex-)degree d_i	number of edges, which are incident to vertex i, so $d_i = \lvert\{e \in E \lvert e = \{i, j\}, j \in V\}\rvert$
k*-star*	sub-graph of G with a vertex i with degree k, all k neighbours of i and all edges incident to i
path of length k	sequence of $k+1, k \geq 0$, different vertices $i_1, ..., i_{k+1}$, where i_l and i_{l+1} are adjacent $\forall l = 1, ..., k$; written as edge sequence: $i_1, e_1 = \{i_1, i_2\}, i_2, e_2 = \{i_2, i_3\}, ..., e_k = \{i_k, i_{k+1}\}, i_{k+1}$
(k*-)cycle*	path (of length k) whose first and last vertex are equal, i.e. $i_{k+1} = i_1$
shortest path	a path between two vertices i, j with the shortest path length
diameter	the maximum of all shortest path lengths

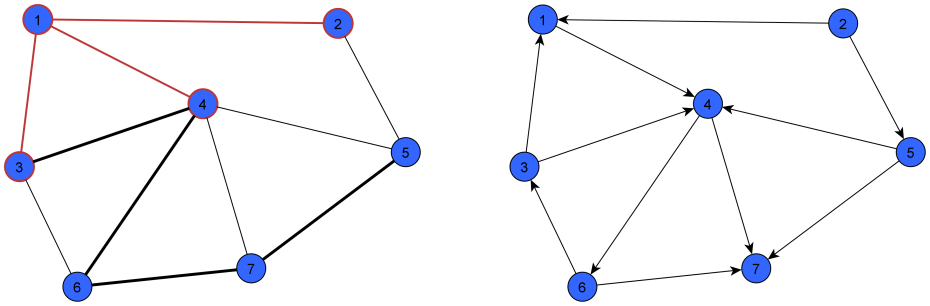
These terms can also be used for directed graphs, but the direction of the edges must be considered. So instead of the vertex-degree for undirected graphs there can be defined an *in-* and an *out-degree* for each vertex, where only edges in or out of vertex i count, i.e.

$$d_i^{(in)} = \lvert\{e \in E \lvert e = (j, i), j \in V\}\rvert \text{ and } d_i^{(out)} = \lvert\{e \in E \lvert e = (i, j), j \in V\}\rvert$$

With these degrees the k*-in-star* is defined as a vertex with $d_i^{(in)} = k$ and $d_i^{(out)} = 0$ and accordingly the k*-out-star* has an in-degree equal to zero and an out-degree equal k. But also *mixed-stars* where edges in and out of the vertex are considered are possible. The aforementioned terms are illustrated in Figure 1.1. Figure 1.1a shows an example of an undirected graph with seven vertices and eleven edges. The vertex set and the edge set for this graph are

$$V = \{1,2,3,4,5,6,7\} \text{ and}$$
$$E = \{\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,4\},\{3,6\},\{4,5\},\{4,6\},\{4,7\},\{5,7\},\{6,7\}\}$$

A path of length 4 exists for instance along the vertices $3-4-6-7-5$, marked with edges in bold in this figure, but the shortest path from vertex 3 to vertex 5 has a length of 2. The degree of vertex 1 is $d_1 = 3$, so this vertex with its neighbours $2, 3, 4$ and the



(a) Example of an undirected graph (b) Example of a directed graph

Figure 1.1: Examples of undirected and directed graphs

edges $\{1,2\},\{1,3\},\{1,4\}$ forms a 3-star, marked with red lines in Figure 1.1a. The graph has 4 3-circles, e.g. $1-3-4-1$ and $4-5-7-4$, and a diameter of 3, because the maximum of all shortest path lengths is 3 (from vertex 2 to vertex 6). Figure 1.1b is an example of a directed graph with the same vertex set as in Figure 1.1a, but the edge set here is

$$E = \{(1,4),(2,1),(2,5),(3,1),(3,4),(4,6),(4,7),(5,4),(5,7),(6,3),(6,7)\}$$

The degrees for vertex 4 are $d_4^{(in)} = 3$ and $d_4^{(out)} = 2$, so this vertex is an example of a mixed-star. A 2-out-star is for instance vertex 2 and vertex 7 is a 3-in-star.

1.2 Examples of networks

Many different fields of life can be modelled with the help of networks. For example in the social domain, where friendships or relationships are explained. There, vertices can be persons, institutions or companies and the edges may represent relations like friendship or blood relationship, but also trade relations or command structures. In most cases social networks are directed graphs, but they can also be modelled with undirected graphs, e.g. for blood relationships.
Another area of application is the traffic system. Here vertices can, for example, stand for cities, which are connected via roads modelled as edges, which can be undirected or directed (for one-way streets for instance).

And also biological problems can be modelled with networks. For example a food web, which describes the "who-eats-whom"-relation between certain animals or plants, can be expressed by a (directed) graph model. Figure 1.2 shows such a food web with six animals and grass as well as arrows, which show which animal eats what. So a directed graph can easily be derived from this picture. For this the vertices represent both animals and grass and the arrows are modelled as directed edges.

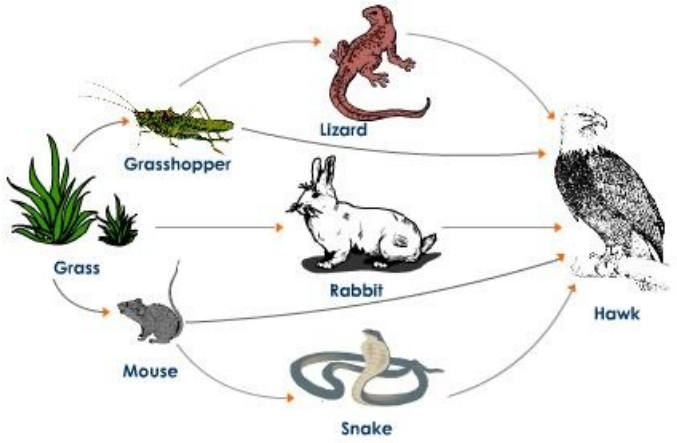
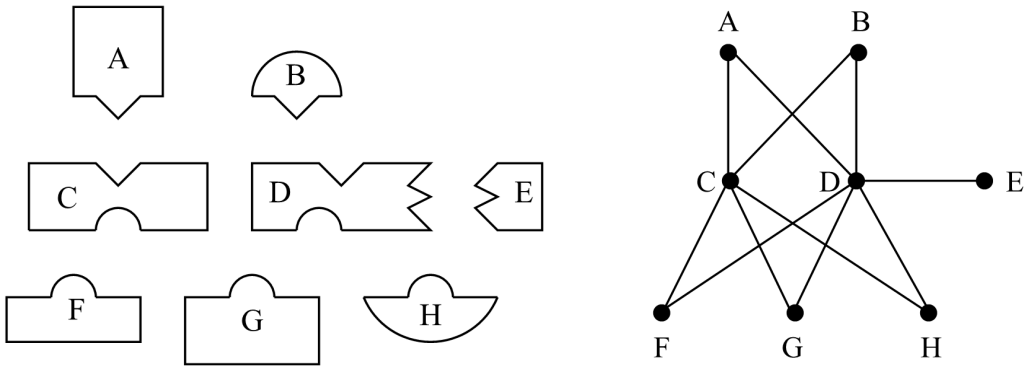


Figure 1.2: A Food Web in a Grassland Ecosystem With Five Possible Food Chains [11]

Other examples of biological networks are brain networks, where the connectivity of the whole brain is examined to get information about the neurobiological interaction, or networks representing interactions between proteins, enzymes or metabolites. The latter can be differentiated into directed networks, such as metabolic or gene regulatory networks (GRN), and undirected networks, e.g. protein-protein interaction networks (PPIN) [4]. PPIN are large, sparse and undirected graphs where the vertices represent proteins and the edges stand for indirect, functional protein interactions like complex, metabolic pathways or regulatory interactions as well as direct physical bindings between proteins [26]. Figure 1.3 shows a PPIN with eight types of proteins (A to H) on the left hand side as schematic representation and on the right hand side as network model, where the proteins can interact with one another if they can be put together like a puzzle. PPIN are used for example to gain more knowledge in human genetics, the prediction of phenotypes and gene functions as well as in research for drug discovery [24].



(a) Schematic representation of the physical basis (b) Modelled Graph

Figure 1.3: Example of a PPIN [9]

2 Random Graph Models

2.1 Simple Random Graph Models

This section will give a short overview of several simple random graph models which are commonly known. First the Erdős-Rényi-Model and the Gilbert-Model as one of the most famous random graph models are described. The second model is the p_1-Model from Holland and Leinhardt, because a generalization of this model, the Exponential Random Graph Models, is explained later (see Section 2.2).

2.1.1 Erdős-Rényi-Model, Gilbert-Model

Paul Erdős and Alfréd Rényi described a very simple random graph model in their work [5] written in 1959. In this model only the number of vertices, n, and the number of edges, m with $0 \leq m \leq \binom{n}{2}$, are given. The *Erdős-Rényi-Model* is therefore also referred to as $\mathscr{G}(n,m)$. With the two parameters n and m, the random graph is constructed by choosing exactly m of the $\binom{n}{2}$ possible edges to be inserted in the graph. So this construction leads to one of the $\binom{\binom{n}{2}}{m}$ undirected simple graphs, which are all equiprobable. Sometimes the number of edges is not constant, but a function of n. Another generalization is to allow parallel edges, which was first studied by Austin et al.
A similar random graph model is the *Gilbert-Model* introduced by Edgar Gilbert also in 1959 in [6]. For this model the number of edges is not given, but a probability $p, 0 \leq p \leq 1$, which says for each pair of vertices independently, whether they are connected or not. Thus the model is related to as $\mathscr{G}(n,p)$. The probability p can, like m in the Erdős-Rényi-Model, be a function of the number of vertices, i.e. $p = p(n)$. In contrast to $\mathscr{G}(n,m)$, the number of edges in the Gilbert-Model is not known in advance. Only the expected number of edges is known as $\binom{n}{2}p$, because m is binomially distributed.

These two classical random graph models can be constructed easily, but are not necessarily suitable for real-life problems. For instance, the Erdős-Rényi-Model has low clustering, unlike social networks, which are normally high clustered [29]. A second disadvantage is the distribution of the vertex degree, which is in such random graphs Poissonian. This stands in contrast to many networks, such as social or neural networks, which appear to have exponential or Gaussian degree distributions [17]. Therefore the two models are only used for comparison in Chapter 3.

2.1.2 p_1-Model

The p_1-*Model* was developed by Paul W. Holland and Samuel Leinhardt [10] to provide a simple and flexible family of probability distributions to analyse simple directed graphs in the field of social networks. It should estimate two important parameters of social networks simultaneously, namely the reciprocation of directed edges and the amount of differential attractiveness exhibited by each vertex. To illustrate these parameters a social network which models the friendship of pupils in a class is considered (see Figure 2.1). The reciprocation counts how many friendships are in both directions and not

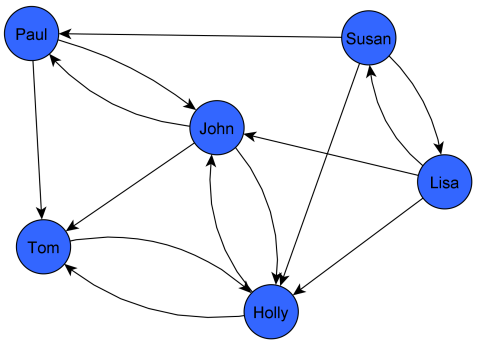


Figure 2.1: Example of a social network for friendship in a class

only from one pupil to another. In the example, there are 4 reciprocated friendships, e.g. between Susan and Lisa or John and Holly. The attractiveness measures, how popular a pupil is, which means how many scholars have this pupil as a friend. Tom, for instance, has an attractiveness of 3, whereas Susan has an attractiveness of 1. The other way around, how many friends a pupil has, is called productivity. In the example, Holly and Paul have both a productivity of 2.
Holland and Leinhardt published their model in 1981 in [10], where the following elaboration and further information can be found.

For social networks two important parameters are the reciprocation between two different vertices i, j, which means that both directed edges (i, j) and (j, i) exist, and the attractiveness of a vertex i, which can be measured with the in-degree of the vertex. With the adjacency matrix of a graph, the number of reciprocated relationships and the number of edges in this graph as well as the in- and out-degree for each vertex can be calculated with the following lemma.

Lemma 2.1: *Let $A = (a_{ij})_{n,n}$ be the adjacency matrix of a simple directed graph, so $a_{ij} \in \{0,1\}, \forall a_{ij} \in A$. The number of reciprocated relationships in this graph is then*

$$r = \sum_{i=1}^{n} \sum_{j=i+1}^{n} a_{ij} a_{ji} \tag{2.1}$$

The number of edges in a graph is

$$m = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \tag{2.2}$$

The in- and out-degree for a vertex i can be calculated for each vertex with the following formulas:

$$d_i^{(in)} = \sum_{j=1}^{n} a_{ji} \tag{2.3}$$

$$d_i^{(out)} = \sum_{j=1}^{n} a_{ij} \tag{2.4}$$

Now, Holland and Leinhardt construct the family of distributions with the help of exponential families of distributions and parameters, that control the probability of observing different values of r and $d_i^{(in)}$ as follows:

Definition 2.2: Let A^* be the set of all possible $n \times n$ adjacency matrices of a simple directed graph, thus $A^* = \{0,1\}^{n,n}$, $x \in A^*$, and X a matrix taking values in A^*. Then the probability function from Holland and Leinhardt is defined as

$$p_1(x) = P(X = x) = e^{\rho r(x) + \theta m(x) + \sum_{i=1}^{n} \alpha_i d_i^{(out)}(x) + \sum_{j=1}^{n} \beta_j d_j^{(in)}(x)} \times K\left(\rho, \theta, \{\alpha_i\}, \{\beta_j\}\right) \tag{2.5}$$

with $\rho, \theta, \alpha_i, \beta_j \in (-\infty, \infty)$.

Here, $r(x), m(x), d_i^{(out)}(x), d_j^{(in)}(x)$ are the values of the corresponding parameters computed from x and $\rho, \theta, \alpha_i, \beta_j$ are parameters that control the probability of observing different values of $r, m, d_i^{(out)}$ and $d_i^{(in)}$. More precisely, ρ controls the reciprocation between two vertices and is therefore named *reciprocity parameter*. θ regulates the number of edges in the graph or in other words the number of ones in the adjacency matrix and is called *density parameter*. α_i governs differences in the distribution of the out-degree, hence it is called *productivity parameter*, and β_j does the same for the in-degree, so it is an *attractiveness parameter*. The function $K\left(\rho, \theta, \{\alpha_i\}, \{\beta_j\}\right)$ is a normalization constant to ensure that the probability sums to 1 over all x.

The derivation of the distribution starts with the definition of pairs $D_{ij} = (a_{ij}, a_{ji})$ for $i < j$, which are called *dyads* in [10] and [28]. There are $\binom{n}{2}$ of such dyads altogether and each can take exactly one of the four values $(0,0), (0,1), (1,0)$ or $(1,1)$. One pair D_{ij} stands for two vertices i, j and the edge(s) between them, as shown in Figure 2.2.

Remark: $D_{ij} = (0,0)$ and $D_{ij} = (1,1)$ are called symmetric dyads, whereas $D_{ij} = (1,0)$ and $D_{ij} = (0,1)$ are asymmetric dyads.

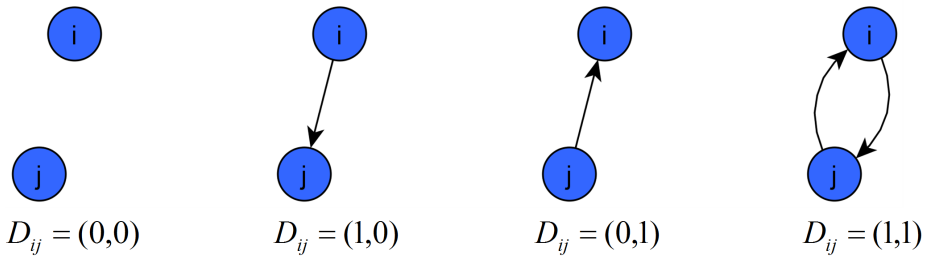


Figure 2.2: All four possible values for D_{ij}

It is assumed that the dyads are statistically independent, which means that the distribution $p_1(x)$ cannot express tendencies toward transitivity, cliquing, hierarchy and so on other than those, which are already implied by tendencies toward reciprocation and differential attraction [10]. The probabilities, which value D_{ij} takes, are referred to as:

$$\begin{aligned} r_{ij} &= P(D_{ij} = (1,1)), \quad i < j^1 \\ s_{ij} &= P(D_{ij} = (1,0)), \quad i \neq j \\ t_{ij} &= P(D_{ij} = (0,0)), \quad i < j^1 \end{aligned} \tag{2.6}$$

The sum over all probabilities must be 1, so the variables defined in (2.6) must satisfy the condition:

$$r_{ij} + s_{ij} + s_{ji} + t_{ij} = 1, \text{ for all } i < j \tag{2.7}$$

The probability $P(X = x)$ can be expressed with these variables in the following way:

$$P(X = x) = \prod_{i=1}^{n} \left(\prod_{j=i+1}^{n} r_{ij}^{x_{ij}x_{ji}} t_{ij}^{(1-x_{ij})(1-x_{ji})} \prod_{\substack{j=1 \\ j\neq i}}^{n} s_{ij}^{x_{ij}(1-x_{ji})} \right) \tag{2.8}$$

with x_{ij} being the values in matrix x. To show on what terms this expression for the probability is the same as in Definition 2.2 the following Theorem is proved.

Theorem 2.3: *The expressions* (2.5) *and* (2.8) *for the probability* $P(X = x)$ *are equal if:*

- $K\left(\rho, \theta, \{\alpha_i\}, \{\beta_j\}\right) = \prod_{i=1}^{n} \prod_{j=i+1}^{n} t_{ij}$ *and*
- $\ln \frac{r_{ij}t_{ij}}{s_{ij}s_{ji}} = \rho$, *for all* $i < j$ *and*
- $\ln \frac{s_{ij}}{t_{ij}} = \theta + \alpha_i + \beta_j$, *for all* $i \neq j$

[1] For $i > j$ the terms r_{ij} and t_{ij} are interpreted as r_{ji} and t_{ji}, respectively.

Proof: For the proof, a third expression for $P(X=x)$ is needed:

$$P(X=x) = e^{\sum_{i=1}^{n}\left(\sum_{j=i+1}^{n}\rho_{ij}x_{ij}x_{ji}+\sum_{\substack{j=1\\ j\neq i}}^{n}\theta_{ij}x_{ij}\right)} \times \prod_{i=1}^{n}\prod_{j=i+1}^{n} t_{ij} \tag{2.9}$$

The following derivation shows, that this expression is the same as (2.8) if $\rho_{ij} = \ln\frac{r_{ij}t_{ij}}{s_{ij}s_{ji}}$ and $\theta_{ij} = \ln\frac{s_{ij}}{t_{ij}}$:

$$\begin{aligned}
P(X=x) &= e^{\sum_{i=1}^{n}\left(\sum_{j=i+1}^{n}\rho_{ij}x_{ij}x_{ji}+\sum_{\substack{j=1\\ j\neq i}}^{n}\theta_{ij}x_{ij}\right)} \times \prod_{i=1}^{n}\prod_{j=i+1}^{n} t_{ij} \\
&= e^{\sum_{i=1}^{n}\left(\sum_{j=i+1}^{n}\ln\frac{r_{ij}t_{ij}}{s_{ij}s_{ji}}x_{ij}x_{ji}+\sum_{\substack{j=1\\ j\neq i}}^{n}\ln\frac{s_{ij}}{t_{ij}}x_{ij}\right)} \times \prod_{i=1}^{n}\prod_{j=i+1}^{n} t_{ij} \\
&= \prod_{i=1}^{n}\left(\prod_{j=i+1}^{n}\left(\frac{r_{ij}t_{ij}}{s_{ij}s_{ji}}\right)^{x_{ij}x_{ji}} t_{ij}\prod_{\substack{j=1\\ j\neq i}}^{n}\left(\frac{s_{ij}}{t_{ij}}\right)^{x_{ij}}\right) \\
&= \prod_{i=1}^{n}\prod_{j=i+1}^{n}\left(\frac{r_{ij}t_{ij}}{s_{ij}s_{ji}}\right)^{x_{ij}x_{ji}} t_{ij}\left(\frac{s_{ij}}{t_{ij}}\right)^{x_{ij}}\left(\frac{s_{ji}}{t_{ji}}\right)^{x_{ji}} \\
&= \prod_{i=1}^{n}\prod_{j=i+1}^{n} r_{ij}^{x_{ij}x_{ji}}\frac{s_{ij}^{x_{ij}}s_{ji}^{x_{ji}}}{(s_{ij}s_{ji})^{x_{ij}x_{ji}}}\frac{t_{ij}^{x_{ij}x_{ji}}t_{ij}}{t_{ij}^{x_{ij}}t_{ji}^{x_{ji}}} \\
&= \prod_{i=1}^{n}\prod_{j=i+1}^{n} r_{ij}^{x_{ij}x_{ji}}s_{ij}^{x_{ij}(1-x_{ji})}s_{ji}^{x_{ji}(1-x_{ij})}t_{ij}^{(1-x_{ij})(1-x_{ji})} \\
&= \prod_{i=1}^{n}\left(\prod_{j=i+1}^{n} r_{ij}^{x_{ij}x_{ji}}t_{ij}^{(1-x_{ij})(1-x_{ji})}\prod_{\substack{j=1\\ j\neq i}}^{n} s_{ij}^{x_{ij}(1-x_{ji})}\right)
\end{aligned}$$

So it is proved that (2.8) $\equiv$ (2.9) under the given conditions. What is left is to show that (2.9) $\equiv$ (2.5) under the conditions given in Theorem 2.3. With the restrictions $\rho_{ij} = \ln\frac{r_{ij}t_{ij}}{s_{ij}s_{ji}} = \rho$ and $\theta_{ij} = \ln\frac{s_{ij}}{t_{ij}} = \theta + \alpha_i + \beta_j$ from the theorem, expression (2.9) becomes:

$$\begin{aligned}
P(X=x) &= e^{\sum_{i=1}^{n}\left(\sum_{j=i+1}^{n}\rho x_{ij}x_{ji}+\sum_{\substack{j=1\\ j\neq i}}^{n}(\theta+\alpha_i+\beta_j)x_{ij}\right)} \times \prod_{i=1}^{n}\prod_{j=i+1}^{n} t_{ij} \\
&= e^{\rho\sum_{i=1}^{n}\sum_{j=i+1}^{n}x_{ij}x_{ji}+\theta\sum_{i=1}^{n}\sum_{\substack{j=1\\ j\neq i}}^{n}x_{ij}+\sum_{i=1}^{n}\alpha_i\sum_{\substack{j=1\\ j\neq i}}^{n}x_{ij}+\sum_{i=1}^{n}\sum_{\substack{j=1\\ j\neq i}}^{n}\beta_j x_{ij}} \times \prod_{i=1}^{n}\prod_{j=i+1}^{n} t_{ij}
\end{aligned} \tag{2.10}$$

If only graphs without self loops are considered[2], which means $a_{ii} = 0, \forall i = 1, ..., n$, it follows with Lemma 2.1:

$$\begin{aligned}
\sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} &= m \\
\sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} = \sum_{j=1}^{n} a_{ij} &= d_i^{(out)} \\
\sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} \beta_j a_{ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} \beta_j a_{ij} = \sum_{j=1}^{n} \beta_j \sum_{i=1}^{n} a_{ij} &= \sum_{j=1}^{n} \beta_j d_j^{(in)}
\end{aligned}$$

for all adjacency matrices A of simple directed graphs. This is also true for matrix x and so (2.10) becomes

$$P(X = x) = e^{\rho r(x) + \theta m(x) + \sum_{i=1}^{n} \alpha_i d_i^{(out)}(x) + \sum_{j=1}^{n} \beta_j d_j^{(in)}(x)} \times \prod_{i=1}^{n} \prod_{j=i+1}^{n} t_{ij}$$

which is the probability from Definition 2.2 if $K\left(\rho, \theta, \{\alpha_i\}, \{\beta_j\}\right) = \prod_{i=1}^{n} \prod_{j=i+1}^{n} t_{ij}$ is satisfied. This means, that expression (2.5) and (2.8) are equal under the conditions from Theorem 2.3. □

For a better understanding of ρ_{ij} and θ_{ij} from the proof, the following equations are considered:

$$\begin{aligned}
e^{\rho_{ij}} = \frac{r_{ij} t_{ij}}{s_{ij} s_{ji}} &= \frac{P(a_{ij} = 1 \wedge a_{ji} = 1) P(a_{ij} = 0 \wedge a_{ji} = 0)}{P(a_{ij} = 1 \wedge a_{ji} = 0) P(a_{ij} = 0 \wedge a_{ji} = 1)} \\
&= \frac{P(a_{ij} = 1 | a_{ji} = 1) P(a_{ij} = 0 | a_{ji} = 0)}{P(a_{ij} = 1 | a_{ji} = 0) P(a_{ij} = 0 | a_{ji} = 1)} \qquad (2.11) \\
e^{\theta_{ij}} = \frac{s_{ij}}{t_{ij}} &= \frac{P(a_{ij} = 1 \wedge a_{ji} = 0)}{P(a_{ij} = 0 \wedge a_{ji} = 0)} \\
&= \frac{P(a_{ij} = 1 | a_{ji} = 0)}{P(a_{ij} = 0 | a_{ji} = 0)} \qquad (2.12)
\end{aligned}$$

From Equation (2.11) follows that, if ρ_{ij} is positive and $a_{ji} = 1$, it is more likely to observe $a_{ij} = 1$. This means, ρ_{ij} controls the force of reciprocation. From the restriction $\rho_{ij} = \rho, \forall i < j$ then follows, that this force should be independent of the vertices i, j. ρ can therefore be interpreted as an average tendency towards reciprocation for all pairs of vertices. The parameter θ_{ij} measures the probability of an asymmetric dyad between vertex i and j if $a_{ji} = 0$. The restriction $\theta_{ij} = \theta + \alpha_i + \beta_j, \forall i \neq j$ implies, that the probability for $P(a_{ij} = 1 | a_{ij} = 0)$ is the sum of a factor for vertex i, a factor for vertex j and an

[2] For social networks this is a common demand, because relationships are never considered between one and the same person.

independent factor.
The weakening of these restrictions leads to a possible generalization of the p_1-Model. Other generalizations can be reached if more than the four given parameters (reciprocity, density, productivity and attractiveness parameter) are considered like in the case of the ERGM described in Section 2.2. Another restriction of the p_1-Models is the assumption, that the dyads D_{ij} are independent. The first models which relax this assumption are the Markov Random Graph Models from Frank and Strauss in 1986 [28]. Hence, the p_1-Models are simple, but easily generalizable, so they are a good starting point for further research.

Simulation of graphs with the p_1-Distribution

This paragraph will show, how a graph can be simulated with the help of the p_1-Model. With the given probability distribution p_1, which means the parameters ρ, θ, α_i and β_j are known, the values for r_{ij}, s_{ij} and t_{ij} are calculated. To get formulas for these parameters, the following system of equations must be solved:

$$\begin{aligned} \rho &= \ln \frac{r_{ij} t_{ij}}{s_{ij} s_{ji}} \\ \theta + \alpha_i + \beta_j &= \ln \frac{s_{ij}}{t_{ij}} \\ 1 &= r_{ij} + s_{ij} + s_{ji} + t_{ij} \end{aligned}$$

From this system the parameters r_{ij}, s_{ij} and t_{ij} can be calculated as:

$$r_{ij} = \frac{e^{\rho+2\theta+\alpha_i+\alpha_j+\beta_i+\beta_j}}{k_{ij}}, \qquad i < j \tag{2.13}$$

$$s_{ij} = \frac{e^{\theta+\alpha_i+\beta_j}}{k_{ij}}, \qquad i \neq j \tag{2.14}$$

$$t_{ij} = \frac{1}{k_{ij}}, \qquad i < j \tag{2.15}$$

where

$$k_{ij} = e^{\rho+2\theta+\alpha_i+\alpha_j+\beta_i+\beta_j} + e^{\theta+\alpha_i+\beta_j} + e^{\theta+\alpha_j+\beta_i} + 1$$

The next step is to simulate one of the four (equiprobable, independent) events of D_{ij} with the help of $r_{ij} = P(D_{ij} = (1,1)), s_{ij} = (D_{ij} = (1,0)), s_{ji} = P(D_{ij} = (0,1))$ and $t_{ij} = (D_{ij} = (0,0))$. These steps are repeated for all $\binom{n}{2}$ pairs $\{i, j\}$ and eventually, the adjacency matrix and with it the graph is simulated. Algorithm 2.1 summarizes the outlined proceeding of simulating a graph.

Algorithm 2.1: Simulation of a graph with the p_1-Distribution

Input: Parameters $\rho, \theta, \alpha_i, \beta_j$ from the distribution
Output: Simulated adjacency matrix

```
Initialize the adjacency matrix A = (a_ij) as an n × n-matrix with all entries equal 0
for i = 1 to n do
    for j = i + 1 to n do
        Calculate r_ij, s_ij, s_ji, t_ij with (2.13)-(2.15)
        Create a pseudorandom number rand from the uniform distribution
        if rand < r_ij then
            Set a_ij = 1 and a_ji = 1
        else if rand < r_ij + s_ij then
            Set a_ij = 1
        else if rand < r_ij + s_ij + s_ji then
            Set a_ji = 1
        end if
    end for
end for
return A
```

2.2 Exponential Random Graph Models

The next Random Graph Model which will be presented is the *Exponential Random Graph Model (ERGM)*. It will become clear why it is called this way at the end of this chapter. Another name for this model is p^**-Model*, because it is a generalization of the p_1-Model from Holland and Leinhardt [28] (see Section 2.1.2). The main development goes back to Frank and Strauss in the 1980s [25]. The ERGM was first developed for social networks and by now it is a common tool in social as well as statistical network analysis and is available in many computer packages to solve problems in this field of mathematics. In the last few years, the ERGM has also been used for modelling biological networks.
The following explanations are based on [20–22, 25]. The notation of the formulas follows [21].

One problem of biological networks is, that they are usually huge – so nobody can examine the whole network. But instead, some local structures of the network are explorable and so the aim of the ERGM is to gather global information from local ones. To get this information, the ERGM models the probability that the observed network is equal to a network, which belongs to a given class of graphs. This probability can be expressed by $P(X = g) = P(g)$, where X is the observed graph and $g \in G$ a graph of the given graph class G. The local structures which are considered for the model are expressed by so called *explanatory variables*, which can be any measurable function from the observed network to the real numbers. E.g. the number of

- edges

- nodes or more precisely nodes with given degree or no neighbours
- k-stars
- k-cycles
- paths of length k

in the graph. Additionally the geometrically weighted sum of these numbers or the diameter of the graph are valid functions. The choice of the explanatory variables depends on what is wanted to be learned about the model, how good the model should be, what could be measured and the available computing capacity. The explanatory variables are referred to as $z_i(g)$ for any graph g and if there are r such variables, these can be summarized in a vector $z(g) = (z_1(g), z_2(g), ..., z_r(g))$. The measured estimate of the expectation of z_i is $< z_i >$. By the definition of expectations, a first condition can be formulated as follows:

$$\sum_{g \in G} P(g) z_i(g) =< z_i > \qquad \forall i = 1, ..., r \tag{2.16}$$

The second condition is the normalization of the probability. So it is

$$\sum_{g \in G} P(g) = 1 \tag{2.17}$$

To make the choice of graph x out of the graph class G as random as possible the maximization of the entropy is used, because the maximum of an entropy is gained, iff the probabilities are equal. For the ERGM the Gibbs' entropy

$$H = -\sum_{g \in G} P(g) \ln P(g) \tag{2.18}$$

is utilized. To maximize this function with conditions the Lagrange multipliers are needed, in this case α for condition (2.17) and $\theta_i, i = 1, ...r$ for the r conditions in (2.16). Now the first derivative of the Lagrange function with respect to $P(g)$ is set to 0:

$$\begin{aligned}
0 &= \frac{\partial}{\partial P(g)} \left(H + \alpha (\sum_{g \in G} P(g) - 1) + \sum_{i=1}^{r} \theta_i (\sum_{g \in G} P(g) z_i(g) - < z_i >) \right) \\
0 &= -(\ln P(g) + 1) + \alpha + \sum_{i=1}^{r} \theta_i z_i(g) && | + \ln P(g) \\
\ln P(g) &= -1 + \alpha + \theta^T z(g) && | e^{\cdots} \\
P(g) &= \frac{e^{\theta^T z(g)}}{e^{1-\alpha}} \\
P(g) &= \frac{e^{\theta^T z(g)}}{\kappa}
\end{aligned} \tag{2.19}$$

with $\theta = (\theta_1, ..., \theta_r)^T$ and $\kappa = e^{1-\alpha}$.
This received equation is the distribution of ERGM similar to the p_1-Distribution in Defi-

nition 2.2 (see Section 2.1.2).
If κ is taken as a normalizing constant, (2.19) can be written as:

$$P(g) \propto e^{\theta^T z(g)} \tag{2.20}$$

This distribution belongs to the exponential family, a class of probability distributions in statistics, and so this Random Graph Model is called "Exponential Random Graph Model".
The Lagrange multipliers θ can be thought of as weights for the explanatory variables z, which means if a θ_i is big, the corresponding variable z_i is important with respect to the classification into the graph class G.
If $P(g)$ in (2.17) is substituted by (2.19), the normalizing constant κ can be written as:

$$\kappa = \sum_{g \in G} e^{\theta^T z(g)} \tag{2.21}$$

And so (2.16) becomes

$$< z_i >= \sum_{g \in G} z_i(g) \frac{e^{\theta^T z(g)}}{\sum_{h \in G} e^{\theta^T z(h)}} \qquad \forall i = 1, ..., r \tag{2.22}$$

With this system of equations with r equations and r unknowns a solution for θ can be found. Note that this solution does not need to exist or be unique, so important questions in this respect are:

- When is there a unique / more than one / no solution?
- If there are more solutions, which should be used?

In [25] Terry formulates the answer for the first question. The following explanation is based on his work.

Theorem 2.4: *The system of equation* (2.22) *always has a solution.*
For this system there is a unique solution for θ_i, if z_i is not constant and $P_\theta(g) \neq 0$ for any θ. If z_i is constant, there are infinite many solutions for θ_i.

Proof: For the proof Terry first introduces the likelihood $L(\theta)$ and the loglikelihood $l(\theta)$ of θ for given graph configurations, which are observed from the real network[3], as follows:

Definition 2.5: Let $\left\{ g_{obs}^{(1)}, g_{obs}^{(2)}, ..., g_{obs}^{(k)} \right\}$ be $k, k > 0$, independent observed graph configurations of the real network and $\theta = (\theta_1, ..., \theta_r)^T$ the vector of weights for the explanatory variables, where each weight can be any real number, in other words $\theta_i \in (-\infty, \infty), \forall i$.

[3] That means the (dynamic) real network is observed over a certain period of time and the configurations are realizations taken during this time.

The *likelihood* of θ is defined as:

$$L(\theta) = \prod_{j=1}^{k} P(g_{obs}^{(j)}, \theta)$$

The *loglikelihood* of θ is simply the natural logarithm of $L(\theta)$:

$$\begin{aligned} l(\theta) &= \ln L(\theta) \\ &= \sum_{j=1}^{k} \ln P(g_{obs}^{(j)}, \theta) \end{aligned}$$

With this definition and the specific probability (2.19) the loglikelihood becomes

$$\begin{aligned} l(\theta) &= \sum_{j=1}^{k} \ln \frac{e^{\theta^T z(g_{obs}^{(j)})}}{\kappa} \\ &= \sum_{j=1}^{k} \left(\theta^T z(g_{obs}^{(j)}) - \ln \kappa \right) \\ &= \theta^T \sum_{j=1}^{k} z(g_{obs}^{(j)}) - k \ln \kappa \end{aligned} \tag{2.23}$$

The first derivative of $l(\theta)$ with respect to θ_i for any $i = 1, 2, ..., r$ then is [4]

$$\begin{aligned} \frac{\partial}{\partial \theta_i} l(\theta) &= \frac{\partial}{\partial \theta_i} \left(\theta^T \sum_{j=1}^{k} z(g_{obs}^{(j)}) - k \ln \kappa \right) \\ &= \sum_{j=1}^{k} z_i(g_{obs}^{(j)}) - \frac{k}{\kappa} \frac{\partial}{\partial \theta_i} \kappa \end{aligned} \tag{2.24}$$

The estimated expectation value $< z_i >$ can be expressed as

$$< z_i > = \frac{z_i(g_{obs}^{(1)}) + z_i(g_{obs}^{(2)}) + ... + z_i(g_{obs}^{(k)})}{k} = \frac{\sum_{j=1}^{k} z_i(g_{obs}^{(j)})}{k} \tag{2.25}$$

and so (2.24) can be written as

$$\frac{\partial}{\partial \theta_i} l(\theta) = k \left(< z_i > - \frac{1}{\kappa} \frac{\partial}{\partial \theta_i} \kappa \right) \tag{2.26}$$

Lemma 2.6: *The values of θ that make $l(\theta)$ stationary are those for which $< z_i > = \frac{1}{\kappa} \frac{\partial}{\partial \theta_i} \kappa$, which means those θ that satisfy condition* (2.22)*.*

[4] Note that κ is a function of θ, in other words $\kappa = \kappa(\theta)$

Proof: $l(\theta)$ is stationary if $\frac{\partial}{\partial\theta_i}l(\theta) = k\left(< z_i > -\frac{1}{\kappa}\frac{\partial}{\partial\theta_i}\kappa\right) = 0$. Because $k > 0$ this means $< z_i >$ must be the same as $\frac{1}{\kappa}\frac{\partial}{\partial\theta_i}\kappa$. From (2.21) follows:

$$\frac{\partial}{\partial\theta_i}\kappa = \frac{\partial}{\partial\theta_i}\sum_{g\in G} e^{\theta^T z(g)} = \sum_{g\in G} z_i(g)e^{\theta^T z(g)} \tag{2.27}$$

And so it must be

$$< z_i >= \frac{1}{\kappa}\frac{\partial}{\partial\theta_i}\kappa = \frac{1}{\kappa}\sum_{g\in G} z_i(g)e^{\theta^T z(g)} = \sum_{g\in G} z_i(g)\frac{e^{\theta^T z(g)}}{\kappa} = \sum_{g\in G} z_i(g)\frac{e^{\theta^T z(g)}}{\sum\limits_{h\in G} e^{\theta^T z(h)}}$$

which is exactly condition (2.22). □

From Lemma 2.6 follows, that if it can be proved that there are θ_i with $\frac{\partial}{\partial\theta_i}l(\theta) = 0$ then these θ_i solve the system of equations (2.22), which means the system is solvable.

Lemma 2.7: *There always exists at least one θ_i that satisfies $\frac{\partial}{\partial\theta_i}l(\theta) = 0$ for all $i = 1, ..., r$.*

Proof: The loglikelihood $l(\theta)$ is bounded above by 0, because the likelihood $L(\theta)$ is the product of probabilities and therefore bounded above by 1. Hence, there exists a biggest value for $l(\theta)$. Furthermore, $l(\theta)$ is defined over all θ_i for $-\infty < \theta_i < \infty$ and is everywhere differentiable. So the loglikelihood must be stationary where it is biggest in any dimension θ_i and so there exists θ_i with $\frac{\partial}{\partial\theta_i}l(\theta) = 0$. □

With Lemma 2.6 and Lemma 2.7 the first part of Theorem 2.4 is proved.
The second statement of the theorem deals with the conditions for a unique solution and for infinitely many solutions. For this, the second derivation of $l(\theta)$ is considered:

$$\begin{aligned}\frac{\partial^2}{\partial\theta_i^2}l(\theta) &= \frac{\partial}{\partial\theta_i}k\left(< z_i > -\frac{1}{\kappa}\frac{\partial}{\partial\theta_i}\kappa\right)\\ &= -k\left(-\frac{1}{\kappa^2}\left(\frac{\partial}{\partial\theta_i}\kappa\right)^2 + \frac{1}{\kappa}\frac{\partial^2}{\partial\theta_i^2}\kappa\right)\end{aligned} \tag{2.28}$$

For the second derivation of κ applies:

$$\frac{\partial^2}{\partial\theta_i^2}\kappa = \frac{\partial}{\partial\theta_i}\sum_{g\in G} z_i(g)e^{\theta^T z(g)} = \sum_{g\in G} z_i^2(g)e^{\theta^T z(g)} \tag{2.29}$$

With (2.27), (2.29), the definition of $P(g)$ and (2.16) the second derivation (2.28) becomes:

$$\frac{\partial^2}{\partial\theta_i^2}l(\theta) = -k\left(-\left(\frac{\sum\limits_{g\in G} z_i(g)e^{\theta^T z(g)}}{\kappa}\right)^2 + \frac{\sum\limits_{g\in G} z_i^2(g)e^{\theta^T z(g)}}{\kappa}\right)$$

$$
\begin{aligned}
&= -k\left(\sum_{g\in G} z_i^2(g)P(g) - \left(\sum_{g\in G} z_i(g)P(g)\right)^2\right) \\
&= -k\left(\sum_{g\in G} z_i^2(g)P(g) - < z_i >^2\right) \\
&= -k\left(\sum_{g\in G} (z_i(g) - < z_i >)^2 P(g)\right) \qquad (2.30)
\end{aligned}
$$

Because a square and a probability are always non-negative, the sum of (2.30) is also non-negative and it is

$$\frac{\partial^2}{\partial \theta_i^2} l(\theta) \leq 0 \qquad (2.31)$$

for all θ. If an explanatory variable z_i is constant, then the estimated value $< z_i >$ is equal to $z_i(g)$ for any graph g and therefore $\frac{\partial^2}{\partial \theta_i^2} l(\theta) = 0$ for all values of θ_i. That means with Lemma 2.7, that there are infinitely many values θ_i which make the loglikelihood stationary and so there are also infinitely many values that satisfy (2.22) (because of Lemma 2.6). Let z_i now be non-constant and additionally $P(g) \neq 0$ for all θ. It follows from (2.30) that $\frac{\partial^2}{\partial \theta_i^2} l(\theta) < 0$ for all values of θ_i. If a function, which is everywhere defined and differentiable, has a negative second derivation in one dimension, this function has a unique maximum in this dimension. Hence, there is a unique solution for θ_i in (2.22) and the second part of Theorem 2.4 is proved. □

If θ is calculated, κ and the probability $P(g)$ can be computed with (2.21) and (2.19), respectively. And with the given probability the network can be simulated (see below). Another possible application is to calculate expectation values $E[\widetilde{z}]$ for graph properties $\widetilde{z}$ that are not measured. So

$$E[\widetilde{z}] = \sum_{g\in G} P(g)\widetilde{z}(g)$$

is the best prediction with respect to the given knowledge of the network. If the values for θ are given, a third application is to use them to estimate the fitting of the observed graph x to these parameters.

The advantages of the ERGM are that several (local) features of a network can be explored simultaneously and the possibility to learn how these local structures form the global network. Another positive aspect is the choice of the explanatory variables, which is very general, flexible and can easily be changed. So the ERGM permits models that are more realistic than for instance the p_1-Model. The various choices of parameters entails also a disadvantage, because with different explanatory variables the gained models are not comparable any more (especially with respect to the fitting). But the main problem of ERGM still is solving the system of equations (2.22) and getting analytic results for the extant variables such as κ or $P(g)$.

Simulation of graphs with ERGM

There are several options to simulate a graph according to the distribution of ERGM. For instance a simulation like for the p_1-distribution described in 2.1.2. But this way is not appropriate in all cases, because a relation between explanatory variables and the adjacency matrix (Equations (2.13)-(2.15) for the p_1-Distribution) must be found, which is not always easy.
Another possibility for simulating uses the probability distribution (2.19). Let g_{ij}^+ be the graph identical to graph g, except for the edge between vertex i and vertex j which definitely exists, and g_{ij}^- the graph identical to graph g, but with the edge between i and j being absent. The probabilities for these graphs are:

$$P(g_{ij}^+) = \frac{e^{\theta^T z(g_{ij}^+)}}{\kappa} \text{ and } P(g_{ij}^-) = \frac{e^{\theta^T z(g_{ij}^-)}}{\kappa} \tag{2.32}$$

The ratio between these probabilities is then:

$$\frac{P(g_{ij}^+)}{P(g_{ij}^-)} = \frac{e^{\theta^T z(g_{ij}^+)}}{e^{\theta^T z(g_{ij}^-)}} = e^{\theta^T (z(g_{ij}^+) - z(g_{ij}^-))} \tag{2.33}$$

Using the ratio has the advantage that it is independent of the normalizing constant κ. Let $d_{ij} = z(g_{ij}^+) - z(g_{ij}^-)$ be the difference in the explanatory variables, which is gained if the status of the edge between i and j is changed from absent to present. Taking the logarithm of (2.33) results in:

$$\ln \frac{P(g_{ij}^+)}{P(g_{ij}^-)} = \theta^T d_{ij} \tag{2.34}$$

This formula can be used to simulate the adjacency matrix and therefore the graph with the given parameters θ and defined explanatory variables, which means that $\theta^T d_{ij}$ can be calculated. If $P(g_{ij}^+) > P(g_{ij}^-)$, which means the edge between i and j is more likely to exist than being inexistent, the ratio is greater than 1 and the natural logarithm of the ratio is greater than 0. Otherwise, if $P(g_{ij}^+) < P(g_{ij}^-)$, the natural logarithm is less than 0 and for $P(g_{ij}^+) = P(g_{ij}^-)$, the natural logarithm is equal to 0. This means, for given explanatory variables and an adjacency matrix, it can be decided, whether an edge between two vertices i, j should exist or not and if it is necessary to adjust the adjacency matrix. Starting with a random matrix for A, the adjacency matrix can successively adapt to the given explanatory variables. Algorithm 2.2 illustrates the described procedure.

Algorithm 2.2: Simulation of a graph with ERGM

Input: Parameters θ from the distribution
Output: Simulated adjacency matrix

```
Initialize the adjacency matrix A = (a_ij) as a random, binary n × n-matrix
while exit conditions not satisfied do
    Choose two vertices i, j ∈ V at random
    Calculate d_ij = z(g_ij^+) − z(g_ij^−)
    Calculate sp = θ^T d_ij
    if sp < 0 then
        Set a_ij = 0
    else if sp > 0 then
        Set a_ij = 1
    end if
end while
return A
```

Remark: If the scalar product $sp = \theta^T d_{ij}$ is equal to 0, the probabilities for the absence and the presence of the edge between i and i are equal. Therefore it does not matter, if a_{ij} is set to 0 or 1 and it can be left at its original value.
Note, that for undirected graphs a_{ji} must have the same value as a_{ij} and has to be set to the corresponding value, too.

In this algorithm, the exit conditions must be defined and can be for instance:

- All different pairs (i, j) were considered.
- A given number of pairs (i, j) was considered.
- The adjacency matrix did not change over a specific period of time.

With Algorithm 2.2 and its formulated exit conditions, the adjacency matrix for the graph and therefore the graph itself will be simulated. The goodness of the fitting in this process depends on the choice of exit conditions: If not enough different pairs (i, j) are considered, the adjacency matrix has not changed much and does not match the explanatory variables.

Special case: Bernoulli-Model

The *Bernoulli-Model* is one of the simplest graph models for an undirected, simple graph. In this model only the number of nodes n and a probability p for the existence of an edge are given. That means, for each of the possible $\binom{n}{2}$ edges it is decided independently with probability p if this edge exists or not. If $m(g)$ is the number of edges of the graph g, then the probability for a Bernoulli-Model can be written as:

$$P(g) = p^{m(g)}(1-p)^{\binom{n}{2}-m(g)} \tag{2.35}$$

The following explanation will show, that the Bernoulli-Model is a specialization of the Exponential Random Graph Model.
An ERGM with only one explanatory variable is considered, where the explanatory variable stands for the number of edges in the network. The number of edges can be calculated from the adjacency matrix A of the network while counting the numbers of entries a_{ij} equal to 1 and dividing by 2. So it is

$$z_1(g) = m(g) = \frac{\{\text{number of 1s in } A(g)\}}{2} \tag{2.36}$$

With (2.36) the normalizing constant κ can be calculated from (2.21):

$$\kappa = \sum_{g \in G} e^{\theta_1 z_1(g)} = \sum_{g \in G} e^{\theta_1 \frac{\{\text{number of 1s in } A(g)\}}{2}} \tag{2.37}$$

The sum in this formula runs through all graphs g, which means through all possible adjacency matrices. The adjacency matrix of an undirected, simple graph is a symmetric binary matrix with $a_{ii} = 0, \forall i$. Let k be the number of entries equal to 1 in such an adjacency matrix. Then this number can vary from 0 to $n^2 - n$ in steps of two. Additionally, there are $\binom{\frac{n^2-n}{2}}{\frac{k}{2}}$ different matrices with exactly k entries equal to 1. With these considerations (2.37) becomes:

$$\kappa = \sum_{\substack{k=0 \\ k \text{ even}}}^{n^2-n} \binom{\frac{n^2-n}{2}}{\frac{k}{2}} e^{\theta_1 \frac{k}{2}} = \sum_{k=0}^{\frac{n^2-n}{2}} \binom{\frac{n^2-n}{2}}{k} e^{\theta_1 k} \tag{2.38}$$

This equation is the summation notation of a special Binomial Formula and with the definition $\binom{n}{2} = \frac{n^2-n}{2}$ the normalizing constant becomes:

$$\kappa = (1 + e^{\theta_1})^{\binom{n}{2}} \tag{2.39}$$

This expression for κ can be substituted into (2.19) and the probability becomes:

$$\begin{aligned} P(g) &= \frac{e^{\theta_1 z_1(g)}}{\kappa} = \frac{e^{\theta_1 z_1(g)}}{(1+e^{\theta_1})^{\binom{n}{2}}} \\ &= \frac{e^{\theta_1 z_1(g)} e^{-\theta_1 \binom{n}{2}}}{(1+e^{-\theta_1})^{\binom{n}{2}}} = \frac{e^{-\theta_1 \left(\binom{n}{2} - z_1(g)\right)}}{(1+e^{-\theta_1})^{\binom{n}{2}}} \\ &= \frac{1}{(1+e^{-\theta_1})^{z_1(g)}} \left(\frac{e^{-\theta_1}}{1+e^{-\theta_1}}\right)^{\binom{n}{2} - z_1(g)} \\ &= \left(\frac{1}{1+e^{-\theta_1}}\right)^{z_1(g)} \left(1 - \frac{1}{1+e^{-\theta_1}}\right)^{\binom{n}{2} - z_1(g)} \end{aligned} \tag{2.40}$$

And if the probability p is set to $p = \frac{1}{1+e^{-\theta_1}}$ a Bernoulli-Model like (2.35) is obtained.

2.3 Small-World Models

The small-world problem dates back to Stanley Milgram, who was the first studying this phenomenon in social networks [16]. He discovered by an experiment, that two randomly chosen people are closely related to each other, despite the fact, that they may be very different[5]. In his experiment, Milgram asked some arbitrarily chosen person living in Nebraska to send a letter to a stockbroker in Massachusetts by passing the letter from person to person. Furthermore, Milgram made the restriction, that the letter may only be send to a person, which is known on a first-name basis. To his surprise he found out, that in average the letter was passed only to six other people before it reached the stockbroker. The conclusion is, that in the world considered as a social network of people connected through friendship or acquaintanceship the average path length between any two people is rather short [17]. Additionally to these short connections between people, most people have a high number of friends or acquaintances, which makes the network highly clustered.
Nowadays the small-world phenomenon can also be found in other fields than social networks, for instance in biological networks, such as the neural network of a worm, spread of diseases or metabolic pathways, and in technical networks, like the power grid of the western United States or airline traffic [17, 29]. All of these small-world networks have the same characteristics, namely a high clustering coefficient, as in regular graphs[6], and a small average path length, like with random graphs [29].
The following sections will describe different models for small-world networks, starting with the first constructed model, developed by Duncan Watts and Steven Strogatz in 1998 in [29].

2.3.1 Watts-Strogatz-Model

Because the small-world networks are a mixture of both regular and random graphs Watts and Strogatz started developing their model from a regular graph and made this more and more "random". For the regular graph they chose a ring lattice with n vertices, each connected to its k, k even, nearest neighbours. In this graph, they rewired each edge with probability p randomly, which leads to a graph, which is not regular any more, but also not completely random. The rewiring process is shown in Algorithm 2.3.

Remark: The parameter k should be set to a value greater than 2, because for $k = 2$ there is a finite probability, that the rewired ring lattice becomes disconnected [18].

[5] In this case, "different" means for example different sex or education, but also physical or social distances.
[6] A *$(k-)$regular graph* is a graph, where all vertices have the same degree, i.e. $d_i = k, \forall i \in V, k \geq 0$.

Algorithm 2.3: Rewiring process for the Watts-Strogatz-Model

Input: $k-$regular ring lattice with n vertices, labelled clockwise with 1 to n and probability $p, 0 < p < 1$

Output: Watts-Strogatz-Model

1: **for** $i = 1$ **to** $\frac{k}{2}$ **do**
2: **for** $j = 1$ **to** n **do**
3: Choose the edge, that connects vertex j to its i-nearest neighbour in a clockwise sense
4: With probability p, reconnect this edge to a vertex chosen uniformly at random from V, but with duplicate edges and self loops forbidden
5: **end for**
6: **end for**

Figure 2.3 shows three different graphs. The left one is a regular ring lattice with 6 vertices, each with 4 neighbours. In the middle, a rewired graph can be seen, where the probability for the reconnection is $p = 0.5$. This graph is an example of the *Watts-Strogatz-Model*. The right graph is a completely rewired and therefore random graph, which has no more characteristics of a regular graph.

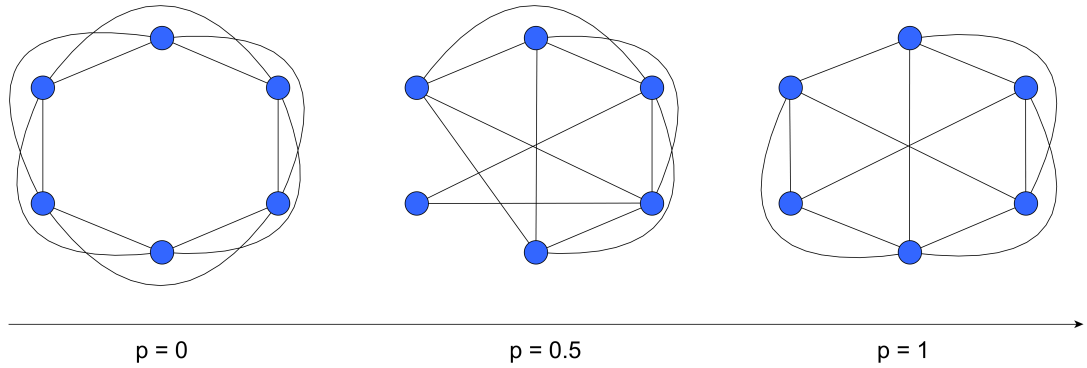


Figure 2.3: Randomly rewired ring lattices according to the probability for reconnection

The characteristic parameters of a small-world model are, as already mentioned, the average path length[7] and the clustering coefficient. The average path length, l, is calculated after Watts and Strogatz by averaging the smallest path length between two vertices over all pairs of vertices and measures the typical separation between two vertices in a network, therefore it has a global character. For random graphs, l scales at most logarithmically with the number of vertices [17] whereas for a ring lattice l is proportional to $\frac{n}{2k}$, so it grows linearly with n. The values for the average path length lie between 1 (for the complete graph) and ∞ (for the edgeless graph).
For the computation of the clustering coefficient, c, a clustering coefficient c_v is defined for all vertices $v \in V$ as the fraction of the number of edges between all neighbours of vertex v and all possible edges between these neighbours. Assuming that v has k_v neighbours $\{1_v, 2_v, 3_v, ..., k_v\}$, then there are $\binom{k_v}{2}$ edges between them possible and c_v

[7] Watts and Strogatz called the average path length in their work the *characteristic path length.*

is equal to

$$c_v = \frac{\{\text{number of edges between all vertices of } \{1_v, 2_v, 3_v, ..., k_v\}\}}{\binom{k_v}{2}} \tag{2.41}$$

The clustering coefficient for the graph then is the average of c_v over all vertices v and quantifies the cliquishness of a typical neighbourhood, so it is a local characteristic [29]. Random graphs do not show clustering, c is therefore small for such graphs. For the three special graphs, edgeless graph, complete graph and ring lattice, the clustering coefficient can be calculated with the following Theorem 2.8.

Theorem 2.8: *For a complete graph the clustering coefficient is* 1*, whereas the edgeless graph has a clustering coefficient equal to* 0*.*
For a ring lattice with k *neighbours per vertex the clustering coefficient is* $c_{rl} = \frac{3(k-2)}{4(k-1)}$*.*

Remark: Note that the clustering coefficients are independent of the number of vertices. The edgeless graph produces the smallest clustering coefficient, whereas the complete graph has the highest value for c, so the clustering coefficient can take values between 0 and 1, i.e. $0 \leq c \leq 1$.

Proof: In a complete graph, all possible edges between all vertices exist and therefore, all possible edges between the neighbours of vertex v exist. This means, that the clustering coefficient for v is $c_v = 1$. This holds for every vertex in the graph and therefore the clustering coefficient for the network is also 1. On the contrary, the edgeless graph has a clustering coefficient equal to 0, because for every vertex v applies $c_v = 0$ as there are no edges between any two vertices.
To proof the second statement of the theorem, a sector of the ring lattice is considered, where vertex v with its k neighbours $1_v, 2_v, ..., k_v$ is shown (see Figure 2.4). To calcu-

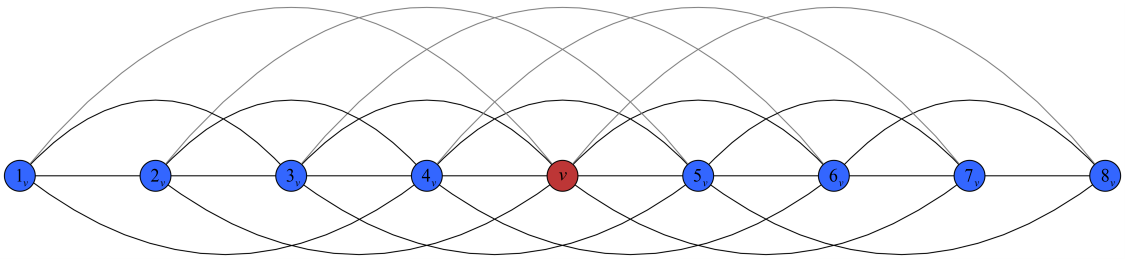


Figure 2.4: Example of sector of ring lattice with $k = 8$

late c_v, the edges between all neighbours of v must be counted. For this, the vertices $1_v, 2_v, ..., k_v$ are considered from left to right and it is counted, how many edges each vertex $i_v, i = 1, ..., k$, has to all neighbours of v, which lie to the right of i_v[8]. All left neighbours of v have $\frac{k}{2} - 1$ such edges each, so in total there are $\frac{k}{2}\left(\frac{k}{2} - 1\right)$ edges. The first right neighbour of v, $\left\{\frac{k}{2} + 1\right\}_v$, has also $\frac{k}{2} - 1$ edges to the right, the second neighbour has $\frac{k}{2} - 2$, the third $\frac{k}{2} - 3$ and so on until the last vertex, k_v, which has no such

[8] To avoid double counting, only the right neighbours are counted.

edges. The sum of all edges of the right neighbours of v is $\left(\frac{k}{2}-1\right)\frac{k}{4}$. So the clustering coefficient is calculated with (2.41) as follows:

$$c_v = \frac{\frac{k}{2}\left(\frac{k}{2}-1\right)+\left(\frac{k}{2}-1\right)\frac{k}{4}}{\binom{k}{2}} = \frac{\frac{3}{4}k\left(\frac{k}{2}-1\right)}{\frac{k(k-1)}{2}} = \frac{3(k-2)}{4(k-1)} \tag{2.42}$$

This equation holds for every vertex of the ring lattice, thus the average over all vertices is equal to (2.42) and so it is $c_{rl} = \frac{3(k-2)}{4(k-1)}$. □

In the Watts-Strogatz-Model, the rewiring probability p is the only selectable variable. To show the effect of p on both parameters, the average path length and the clustering coefficient, an experiment, as described in [29], was conducted. Here, based on a ring lattice with 1000 vertices and a vertex degree of 10, i.e. $k = 10$, Watts-Strogatz-Models were produced for different probabilities and the average path length as well as the clustering coefficient were measured according to p. The following values were chosen as probabilities:

$$p \in \{0.0001, 0.0002, 0.0003, 0.0006, 0.001, 0.002, 0.003,$$
$$0.006, 0.01, 0.02, 0.03, 0.06, 0.1, 0.2, 0.3, 0.6, 1\}$$

To avoid random effects, 20 models are created for each probability, whose results were averaged. Afterwards, the values for $l(p)$ and $c(p)$ were normalized by $l(0) = \frac{555}{11}$ and $c(0) = \frac{2}{3}$, respectively, the values for the ring lattice. Figure 2.5 shows the results of this experiment. This diagram shows, that the average path length as well as the clustering

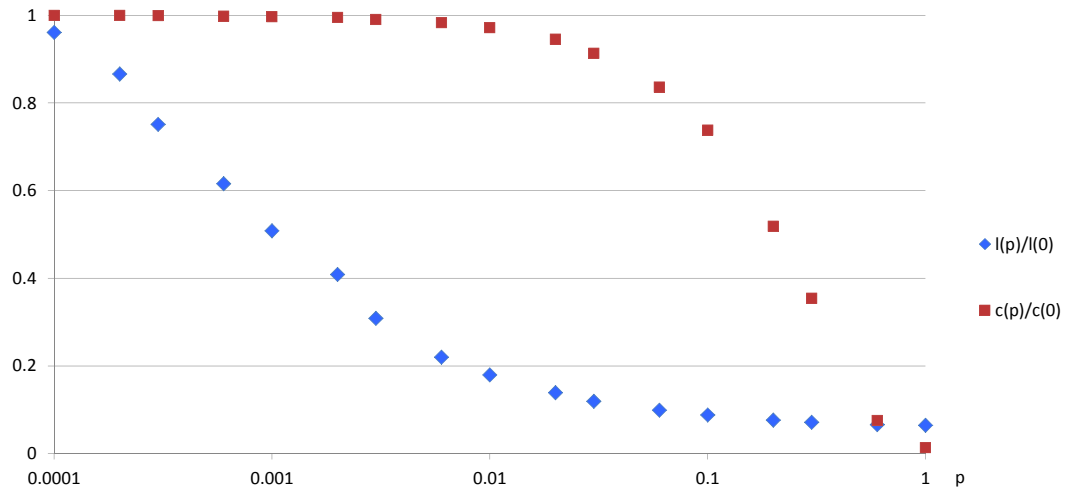


Figure 2.5: Normalized average path length $\frac{l(p)}{l(0)}$ and clustering coefficient $\frac{c(p)}{c(0)}$ plotted against the probability p for rewiring with logarithmic scale

coefficient become smaller with greater values for p, but the decrease of $l(p)$ is much faster than the decrease of $c(p)$. This means, the immediate drop of $l(p)$ is gained by rewiring just a few edges in the ring lattice, because these new "long-range" edges are sufficient to build short cuts in the graph, which will lead to a much lower path length. In

contrast, the new edges do not change the clustering of the ring lattice dramatically, so the clustering coefficient stays nearly the same for small p.
The result of this experiment is the choice of parameter p: Because a small average path length and a high clustering coefficient is desired for small-world models, the rewiring probability should be chosen between 0.01 and 0.1 (cf. Figure 2.5).

Hence, the graphs constructed by Watts and Strogatz can produce good models for small-world networks in the sense of small average path length and high clustering coefficient. A disadvantage of the Watts-Strogatz-Model can be the nearly constant vertex degree, which fits many small-world networks, but not for instance the world-wide web [17].

2.3.2 Kleinberg-Model

Milgram showed in his experiment, that two randomly chosen people are closely related, which means that there exist short chains of acquaintances linking together persons, who do not know each other. In the experiment, the people, who received the letter, found the chains without knowing the complete network of acquaintanceship. So Jon Kleinberg asked, how two randomly chosen persons are able to find short chains of acquaintances that link them together [14]. He thought, that there had to exist "cues" in the social network, which guided the letter quickly from the sources in Nebraska to the target (the stockbroker in Massachusetts). Therefore, Kleinberg's aim was to create a small-world model, on which a simple algorithm can find a short path between two randomly chosen persons or more generally nodes, source and target, only by using local information.

The *Kleinberg-Model* described in [14] starts with a two-dimensional grid with N^2 vertices placed in an $N \times N$ square as shown in Figure 2.6a. The vertices are labelled according to their position in the grid, starting in the upper left corner, so it is $V = \{(i,j)|i \in \{1,2,3,...N\}, j \in \{1,2,3,...N\}\}$. Between those vertices, a distance is defined as follows:

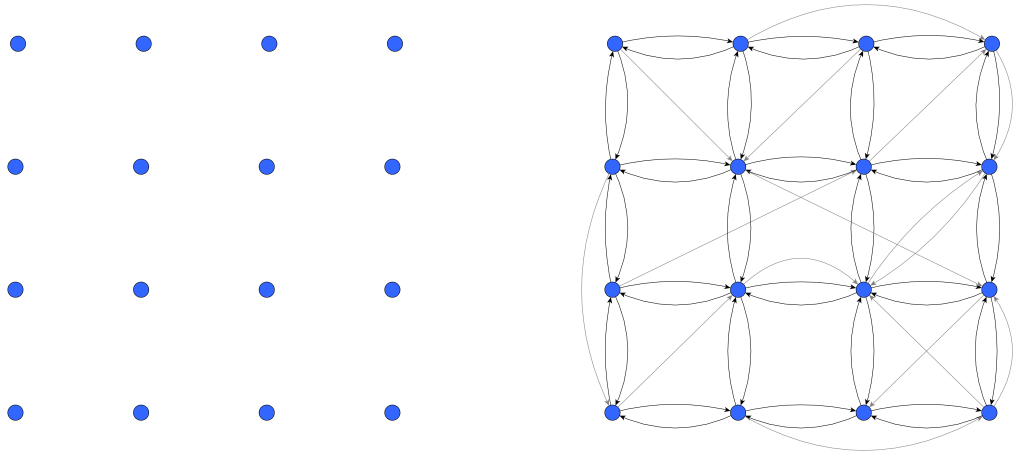
Definition 2.9: In a two-dimensional grid with vertex set $V = \{(i,j)|i \in \{1,2,3,...N\}, j \in \{1,2,3,...N\}\}$, the *lattice distance* between two vertices (i,j) and (k,l) is

$$d((i,j),(k,l)) = |k-i| + |l-j| \tag{2.43}$$

Remark: The lattice distance can be interpreted as number of lattice steps needed to get from vertex (i,j) to vertex (k,l) and vice versa.
This distance is also known as *Manhattan distance*.

The construction of the model continues with the addition of directed edges to the grid. These edges are modelled on social networks, where people have many friends or

acquaintances, which are near to them in the sense of physical distance, and just a few contacts, which live far away from this person. For an arbitrary parameter $p \in \mathbb{N}$, each vertex $u \in V$ is connected to all vertices, which have a lattice distance from u at most p, with directed edges. This means, there is a directed edge from u to v iff $0 < d(u,v) \leq p$. These neighbours of u are called *local contacts*. Additionally, each vertex u is connected to $q \in \mathbb{N}_0$ other vertices, so called *long-range contacts*, with directed edges. Thereby the long-range contacts are chosen with a probability proportional to $d(u,v)^{-r}$, where $r \in \mathbb{R}_{\geq 0}$ is a third selectable parameter. To obtain a probability, $d(u,v)^{-r}$ must be divided by the normalizing constant $\sum_{v \in V \setminus \{u\}} d(u,v)^{-r}$. Figure 2.6b shows an example of the Kleinberg-Model, which can be gained from the two-dimensional grid on the left side if $p = 1$ and $q = 1$. Here, the directed edges between local contacts are marked with black arrows and the long-range contacts are connected with grey arrows.



(a) Two-dimensional grid with $N = 4$

(b) Kleinberg-Model with $N = 4, p = 1$ and $q = 1$

Figure 2.6: Construction of the Kleinberg-Model

The parameter r controls the selection of the long-range contacts according to the lattice distance. If $r = 0$, the long-range contacts of a vertex are chosen independently of their distance to this vertex. This uniform distribution can be found in the Watts-Strogatz-Model, where the endpoints of the rewired edges are also chosen independently. Therefore, the Kleinberg-Model can be seen as a generalization of the Watts-Strogatz-Model [17], where a two-dimensional grid is used as regular graph instead of a ring lattice. If r increases, the long-range contacts get more and more closer to the corresponding vertex. This makes the generated graph highly clustered, but there will be less short cuts in the graph. Kleinberg proved in his work [14], that $r = 2$ is the only value, for which an algorithm, which uses only local information, exists, that finds a path between source and target whose length is polynomial in $\log N$. For values $r \neq 2$, each such algorithm finds only paths with length polynomial in N. Thus, for the construction of a Kleinberg-Model, the parameter r should be set to 2.

Remark: The local information used in an algorithm are according to Kleinberg [14]:

- the set of local contacts among all vertices, which means the grid-structure as well as the parameter p
- the location of the target in the grid and
- the location as well as the set of all long-range contacts of all vertices, that already received the message

Thus, the algorithm has no knowledge about the long-range contacts of vertices, which have not got the message yet.

The algorithm used in [14] to find a path in a Kleinberg-Model constructed with $p = q = 1$ and $r = 2$ is a greedy heuristic [15] and has the following structure: Starting in source s, a contact of s is chosen, which has the shortest lattice distance to target t. The message is sent to this vertex, say x_1, and further to a contact of x_1, which has the shortest lattice distance to t. In this way, the message is sent through the graph until a vertex x_i is reached, who has t as a contact. The last step is to send the message to vertex t. To improve the performance of the algorithm, the Kleinberg-Model is not completely initialized. Only the grid and the local contacts are constructed at first, but the long-range contacts of a vertex are not inserted until the algorithm reaches this vertex. This conforms with the demand for local information, which should be used in the algorithm, because the long-range contacts of vertices, which have not received the message yet, are not known since they have not been inserted into the model yet.
To show the effect of the exponent r on the model, an experiment was conducted where the average number of steps needed to send a message from a source to a target was measured as a function of r. In this experiment a Kleinberg-Model with $N = 100$ and $p = q = 1$ was generated. The value for r varies from 0 to 10 in steps of 0.5, i.e.

$$r \in \{0, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9, 9.5, 10\}$$

The source and the target are set to the upper left and lower right corner, respectively, this means $s = (1,1)$ and $t = (N,N)$. The algorithm used for finding a path between s and t is as described above. To avoid random effects, 20 models were created for each exponent r and the number of steps needed to get from s to t were averaged. The result of the experiment can be seen in Figure 2.7. This diagram shows, that for $r \leq 2$ the number of steps is nearly the same and small. For values between 2 and 4, the path length between s and t increases very fast. For $r \geq 4$, the number of steps is much higher than for $r \leq 2$, but it does not change dramatically any more. The experiment shows the effect of r on the number of steps needed to find a path between a source and a target in tendency, but not the exact results proved by Kleinberg in his work.

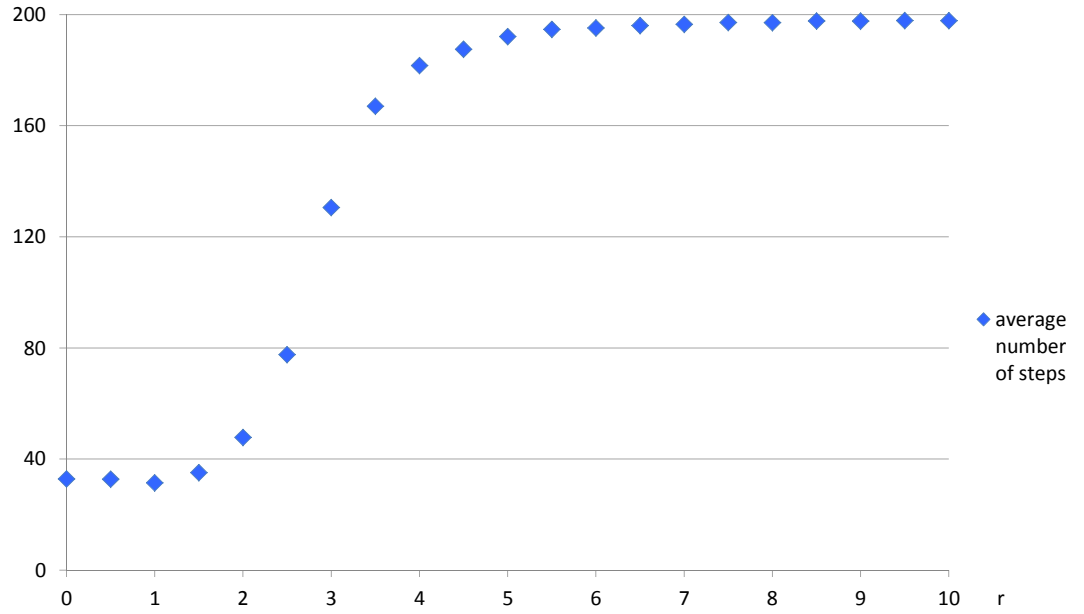


Figure 2.7: Average number of steps needed to deliver a message from s to t plotted against the exponent r for long-range contacts

The Kleinberg-Model can be generalized by using a k-dimensional grid instead of a two-dimensional grid for $k \in \mathbb{N}, k > 2$. For these models, the exponent r should be set to $r = k$ [14]. Another modification of the model can be gained by replacing the lattice distance with a different distance, for instance the Euclidean distance $d((i,j),(k,l)) = \sqrt{(k-i)^2 + (l-j)^2}$.
This model shows, that the small-world effect involves more than the existence of short paths [17]. Moreover, there are structural cues, which help finding these short paths and Kleinberg pointed out, that these cues depend on the structure of long-range contacts. The Kleinberg-Model is a good model for routing problems, where only local information is available [14]. Such problems are for instance the navigation of a robot in an unknown area or finding a path in a communication network with as less information as possible.

2.3.3 Further Small-World Models

Because the Watts-Strogatz-Model was the first one developed for small-world networks, many other models are based on this model. Some of these enhancements will be presented in the following section.

As elaborated in 2.3.1, a problem of the Watts-Strogatz-Model is the possible disconnectedness of the constructed graph. If the model, which is created by rewiring edges, has more than one component, the average path length is infinite, because there are at least two vertices, which are not connected through a path and therefore the path length

between them is infinite. To avoid this, Mark Newman and Duncan Watts proposed the insertion of edges into the ring lattice instead of rewiring the edges [18]. The inserted edges are chosen at random like the position of the rewired edges in the Watts-Strogatz-Model, which means the created short cuts will stay the same. The only difference is, that the edges, which should be rewired, are not removed from the ring lattice. This follows, that if the initial graph (the ring lattice) is connected, the new graph is also connected, because there are only edges added and not removed. Thus there exists a path between any two vertices in the model and therefore the average path length will be finite.
A new idea is to combine both models, the Watts-Strogatz-Model and the model suggested by Newman and Watts. For this, a second probability, named q, is needed, which declares, whether the original edges shall be removed during the rewiring process. The extended algorithm, which describes all three models, can be found in Algorithm 2.4.

Algorithm 2.4: Extended Watts-Strogatz-Model

Input: $k-$regular ring lattice with n vertices, labelled clockwise with 1 to n and two probabilities $p,q, 0 < p,q < 1$
Output: Extended Watts-Strogatz-Model

```
for i = 1 to k/2 do
    for j = 1 to n do
        Choose the edge, that connects vertex j to its i-nearest neighbour in a clockwise sense
        With probability p, insert an edge from j to a vertex chosen uniformly at random from V, but with duplicate edges and self loops forbidden
        With probability q, remove the chosen edge
    end for
end for
```

Remark: Note, that for $q = 1$ a Watts-Strogatz-Model is gained, whereas for $q = 0$ a model according to Newman and Watts is created.

Kasturirangan described another model in his work [13], where edges are added to a given graph, too. In contrast to Newman and Watts, these edges are not chosen randomly, but with the distribution of so called *length scales*.

Definition 2.10: Let G be a graph with n vertices, $\text{dist}_G(f,g)$ the distance between two vertices f,g in G and W a set of new edges added to G. The distance of an edge $e_W = \{f_e, g_e\} \in W$ is $\text{dist}_G(e_W) = \text{dist}_G(f_e, g_e)$. The *distribution of length scales* in W, written as $D(W)$, is measured by the function

$$D : W \to (1,\infty) : e_W \mapsto D(e_W) = \text{dist}_G(e_W)$$

With this distribution, Kasturirangan defined a new class of graphs as follows:

Definition 2.11: Let H be a graph with n vertices. A graph G is a *multiple scale graph*, if it is obtained by adding many edges with different length scales to H, i.e.:

$$\exists r \gg 0 : \exists \text{length scales } l_i, i = 1,2,...,r : 0 < l_1 \ll l_2 \ll ... \ll l_r \leq n \text{ and } l_i \in D(W)$$

Kasturirangan proved, that the insertion of many edges with many different length scales to any graph leads to a decrease of the average path length. So if this is done to a regular graph, both characteristics of a small-world graph (a small average path length and a high clustering coefficient) are gained [13]. Therefore the multiple scale graph is also a good model for small-world problems.

Another enhancement of the Watts-Strogatz-Model was also suggested by Kasturirangan in [13]. Instead of adding edges to a graph, he proposed adding a few vertices, so called *hubs*, which are connected to many, randomly chosen vertices from the original graph. An example of this model is given in Figure 2.8. These hubs involve a decrease

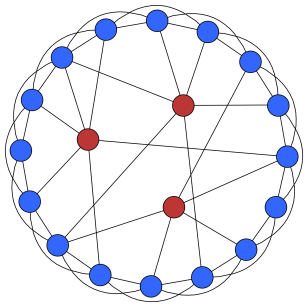


Figure 2.8: Example of a ring lattice with hubs (red vertices)

of the average path length, because they create short cuts between two randomly chosen vertices. Even if just one sufficiently highly connected vertex is added, the new graph exhibits the small-world effect [17]. The maximum decrease of the average path length can be achieved, if one vertex is added and connected to each vertex of the ring lattice. With this hub, any two vertices are connected with a path of length at most two. Yet, this model is not appropriate for every problem [13]. For instance for a communication network, where most of the messages will be guided over this hub. This may lead to an overload in this vertex, which implies, that the communication speed will be low if many messages arrive at the hub simultaneously. Additionally, the failure of the hub results in a huge increase in the average path length. Therefore the difficulty of this model lies in the choice of the hubs, that is the number of hubs as well as the connection between the hubs and the vertices of the ring lattice.

3 Construction of Models for PPIN

This chapter covers the testing of how well the described models (see Chapter 2) fit to a concrete biological network, namely the protein-protein interaction network of Escherichia coli (E. coli), which is explained in Section 3.1. The construction of an Exponential Random Graph Model and a small-world model are described in 3.2 and 3.3, respectively. Finally, these two models as well as the Simple Random Graph Models of Erdős-Rényi and Gilbert are compared with respect to the fitting of the models to the PPIN of E. coli.

3.1 Biological Background

To test the random graph models on a biological network, the protein-protein interaction network (PPIN, see 1.2) of the bacterium Escherichia coli (E. coli) was chosen. E. coli is a microorganism, which is often used for research in system biology. The reason for this is twofold: On the one hand, E. coli is a well-researched bacterium and much data and practical applications are available for it. On the other hand, E. coli is important for the human body, as it can be found in the intestinal flora where it prevents the spreading of harmful microorganisms. Lately it is used more and more often in the production of important drugs, so called biopharmaceuticals. Nevertheless there are also dangerous, disease-causing variants of E. coli, for example EHEC. [3]
The protein-protein interaction network of E. coli was obtained from a biological database named STRING (Search Tool for the Retrieval of Interacting Genes/Proteins) database[9], which was first released in 2000 [12]. The current version 9.0 of the database contains more than five million proteins from over 1100 completely sequenced organisms and their protein interactions [24]. The interactions are derived from high-throughput experimental data, the mining of other databases and literature as well as from predictions based on genomic context analysis [27]. This means, there are different types of interactions between proteins in the database corresponding to the method, how these interactions have been verified. These different interactions are ranked by benchmarking them against a common reference set of trusted, well-known protein connections [27]. For example, if an interaction between two proteins is discovered by one or more experiments, the score of this connection will be higher than the score of an interaction, which was only gained through text mining. Consequentially, the predicted connections get the lowest score.

For this master thesis, only PPIN of E. coli were used whose protein interactions were obtained from experimental data, which means that the connections between proteins are assured. In these networks some proteins, so called *targets*, were chosen to be

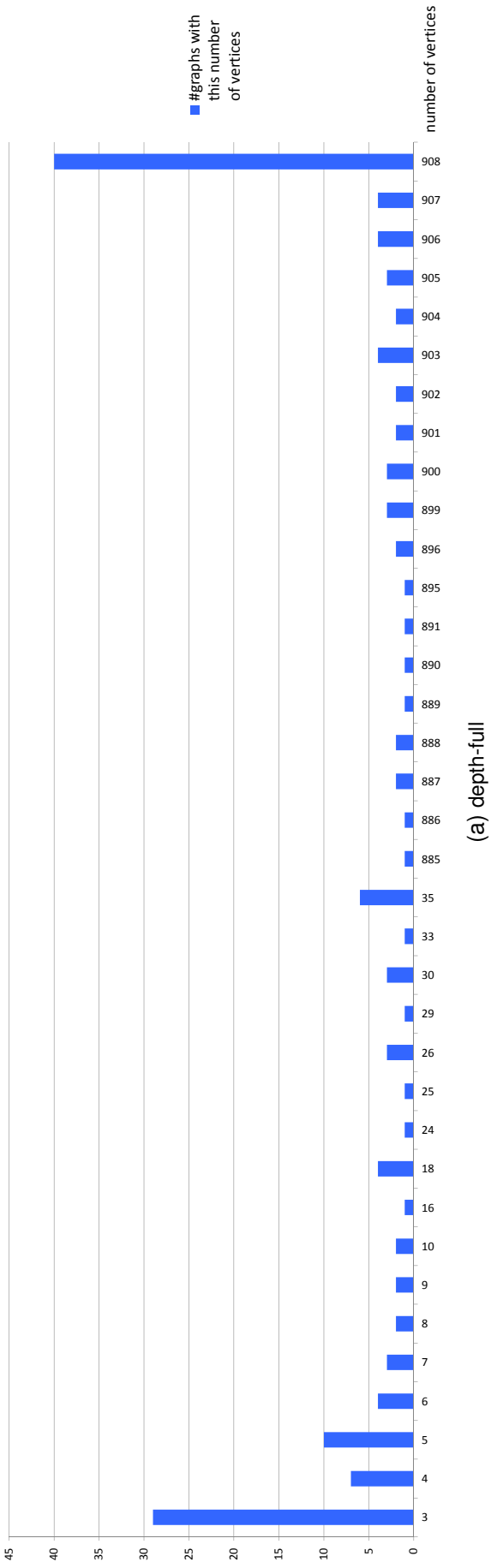
[9] available at http://string-db.org/

removed from the network, splitting the respective graph into at least two subgraphs. These subgraphs were then used for the construction of random graph models. Additionally to these full networks, graphs were created containing only proteins, which have a maximum distance of five connections to the target. From these networks, the target was removed as well. Thus there are two types of PPIN to test, one with full depth from the target and one with a depth of only five. For full depth, 78 targets were chosen, which produced 159 networks. The size of these graphs differs a lot as there are networks with only 3 vertices up to networks with 908 vertices and moreover, there are no graphs with a number of vertices between 36 and 884. The complete distribution of the number of vertices is given in Figure 3.1a. Additionally, there are 1147 graphs with a depth of five gained from 473 targets. The biggest network for this type has 346 vertices and all 1147 networks contain a total of 996 unique proteins. The number of graphs for all occurred values of n can be seen in Figure 3.1b. Table 3.1 shows a summary of the considered networks.

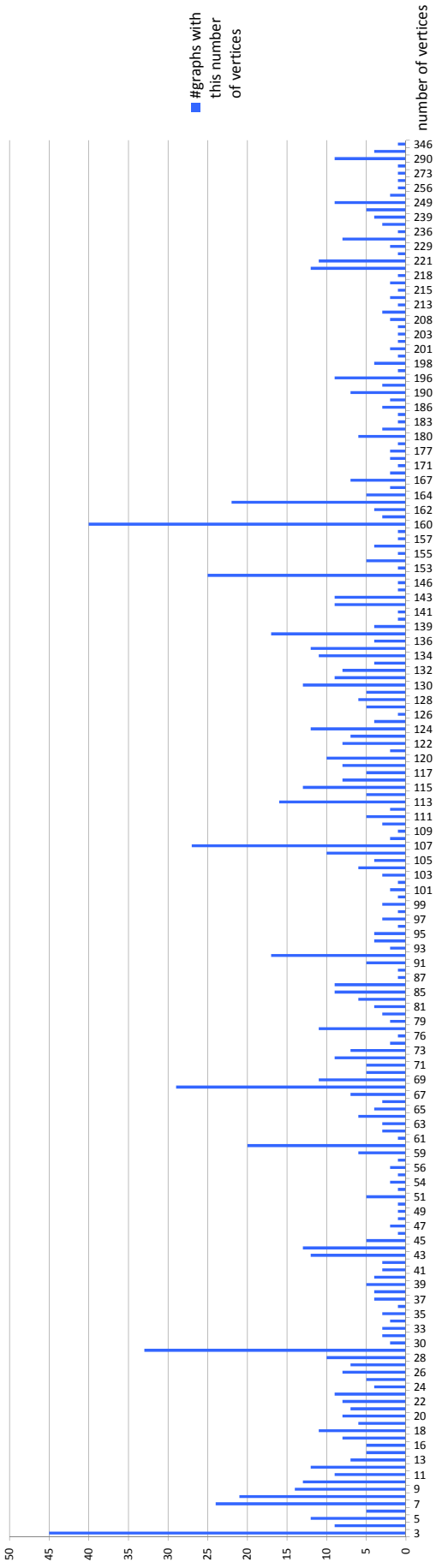
Table 3.1: Summary of considered networks

type of networks	**depth-full**	**depth-5**
number of graphs	159	1147
number of chosen targets	78	473
number of different proteins	980	996
range of number of vertices	3–908	3–346

Remark: In the following sections, the networks created with full depth are referred to as depth-full whereas the term depth-5 corresponds to graphs, which were gained by only considering a depth of five.



(a) depth-full



(b) depth-5

Figure 3.1: Number of graphs plotted against the number of vertices

3.2 Construction of an ERGM

To create an Exponential Random Graph Model for a given network, at first the explanatory variables $z(g)$ must be defined. For the PPIN, the number of edges and triangles in the graph as well as the degree for each vertex was chosen. The probability distribution is then:

$$P(g) = \frac{e^{\theta m(g) + \rho tri(g) + \sum_{i \in V} \alpha_i d_i(g)}}{\kappa} \tag{3.1}$$

with $m(g)$ the number of edges in graph g, $tri(g)$ the number of triangles in g and $d_i(g)$ the degree of vertex $i, i \in V$, in graph g with vertex set V.
The parameters θ, ρ and $\alpha_i, i \in V$, must then be calculated as described in 2.2. For this, the normalizing constant κ has to be known, which is impossible in most cases for graphs with a number of vertices greater than 6 [23]. Therefore, the parameters cannot be calculated exactly. A possible way around this is to estimate the parameters instead of calculating the exact values. There are several software packages available to estimate parameters of ERGM, for instance the "statnet" suite for the "R statistical computing environment" [21], which was used in this master thesis. The software suite "statnet" contains software tools for the analysis, simulation and visualization of network data, which were written in a combination of R and (ANSI standard) C [8]. It runs in the free software environment for statistical computing and graphics, R [19], and uses the package "network" of R. One package of "statnet" is "ergm", which calculates user-defined explanatory variables for a given network using *Markov Chain Monte Carlo Maximum Likelihood Estimation* (MCMC MLE). For further information on MCMC MLE see for example [7] or [21]. To use "ergm" in R, the following commands have to be entered:

```
%Load needed library
> library("statnet")
%Define a network from a matrix
> m <- matrix(c(0,1,0,0,1,1,0,0,0,1,0,0,0,1,1,0,0,1,0,1,1,1,1,1,0),
ncol=5, nrow=5, byrow=TRUE)
> n <- network(m, directed=FALSE)
%Execute ERGM with given explanatory variables
> results <- ergm(n ~ edges + triangles + sociality(base=0))
```

Figure 3.2: Input commands for R

At first, the library "statnet" has to be loaded, which provides the package "ergm", amongst others. The next two commands create a matrix and with it a network using the package "network" from R. In this example, an undirected graph is constructed from a 5×5-matrix. The last step is the estimation of the explanatory variables of the defined network. For this purpose, "ergm" provides many different explanatory variables for both undirected and directed graphs. The used parameters *edges*, *triangles* and *so-*

ciality in this example represent the explanatory variables $m(g)$,$tri(g)$ and $d_i(g)$ from (3.1). The R script with the resulting output can be found in Appendix A.1.
While using R, two problems occurred: One problem was, that there was not enough memory to create huge networks, so the graphs from depth-full could not be used for calculating the parameters. Instead, only networks from depth-5 were considered. The second problem was, that sometimes no values were calculated for a network, which is due to the fact, that "statnet" is still experimental and not guaranteed to be stable or fully functional. Therefore the graphs, for which these problems occurred, could also not be used for calculating. Altogether, 913 of 1147 graphs of depth-5 were used to estimate the values for the explanatory variables.
The parameters for each network were estimated and the values for all networks were averaged. The average as well as the minimum and maximum of the calculated values for each explanatory variable can be found in Table A.1 from Appendix A.2.

To test the estimated values, Algorithm 2.2 was used to create an ERGM for each network from depth-5, which had not been used for the calculation of the explanatory variables. Altogether, 234 networks were used for testing. The values for each parameter were set to the averaged calculated values from "statnet" (see row "avg" in Table A.1). The algorithm was executed with different exit conditions. For this, all pairs of vertices were considered once, twice, three and four times. Additionally, two methods of handling the changes in the adjacency matrix were executed:

- The change is conducted in place. This means, the calculation for the next pair of vertices is executed on a new adjacency matrix.
- The change is stored until all pairs of vertices are considered. This means, the adjacency matrix does not change before a whole run[10] is executed.

For each model a quality measure was calculated, which quantifies the fitting of the model to the original network. The quality measure was defined as the sum of the difference in the vertex-degrees between model and original network (QM_{deg}) and the difference in the number of edges (QM_m). This means, the quality measure $QM^{(ERGM)}$ is:

$$\begin{aligned} QM^{(ERGM)} &= QM_{deg} + QM_m \\ &= \sum_{i=1}^{n} |d_i(orig) - d_i(model)| + |m(orig) - m(model)| \end{aligned} \tag{3.2}$$

with $d_i(orig), d_i(model)$ the degree of vertex i and $m(orig), m(model)$ the number of edges in the original PPIN and in the model, respectively.
The averaged quality measures for the different number of runs and the two methods for changing the adjacency matrix are listed in Table 3.2. This table shows, that more repetitions do not improve the fitting and that there is no remarkable difference between

[10] A run means in this case, that all pairs of vertices were considered once.

Table 3.2: Averaged values of $QM^{(ERGM)}$ according to number of runs

runs	1	2	3	4
immediate change	2560.25	3997.69	4118.21	4303.14
stored change	2552.21	4163.18	4216.52	4079.93

the immediate change of an entry in the adjacency matrix and the deferred change after a whole run. This means, it is sufficient to consider each pair of vertices once. The share of the single differences QM_{deg} and QM_m in the quality measure can be seen in Figure 3.3. The diagram shows, that the difference in the vertex-degrees holds the main part, whereas the difference in the number of edges is just about a quarter of $QM^{(ERGM)}$.

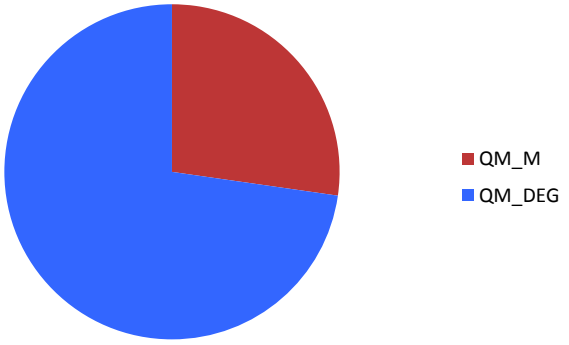


Figure 3.3: Partition of $QM^{(ERGM)}$

Additionally, Exponential Random Graph Models were created, where the values for the explanatory variables are set to the average of the calculated values, which are unequal to $\pm\infty$ (see row "$\text{avg}_{\text{no inf}}$" in Table A.1). For this, some graphs had to be skipped for testing, because they have explanatory variables, which have no such average. Accordingly, only 225 graphs were left for testing. However, the resulting quality measures were much worse than those, where the pure averages were used as parameters. This follows, that for the construction of an ERGM the pure average of the estimated values should be used, but with the addition that if an infinite value occurs, it must be set to a sufficiently high value, which can be used for the calculation of the average (in this case $\pm\infty$ was set to ± 1000).

3.3 Construction of a Small-World Model

Before the small-world models for the PPIN were constructed, the networks were verified whether a small-word model is applicable. This means at first it was analysed, if the characteristics of a small-world network (small average path length and high clustering coefficient) are given with the PPIN of E. coli. For this, the average path length and the clustering coefficient were calculated for each network and summarized for graphs with

a similar number of vertices. The resulting values for depth-full and depth-5 are given in Table 3.3 and Table 3.4, respectively. The first line in Table 3.3 shows for example, that all networks with a number of vertices between 3 and 10, of which there are 59, have in average an average path length of 1.601 and a mean clustering coefficient of 0.186. The smallest average path length for these 59 networks is 1.3, whereas the greatest value is 3.667.

Table 3.3: Small-world characteristics for depth-full

graph class		**average path length**			**clustering coefficient**		
range of n	#graphs in class	min	max	average	min	max	average
3–10	59	1.300	3.667	1.601	0.000	0.867	0.186
16–35	21	1.824	6.760	3.774	0.064	0.874	0.560
885–908	79	5.400	5.902	5.818	0.453	0.467	0.458

Table 3.4: Small-world characteristics for depth-5

graph class		**average path length**			**clustering coefficient**		
range of n	#graphs in class	min	max	average	min	max	average
3–10	143	1.000	2.844	1.925	0.000	1.000	0.180
11–20	71	1.287	3.626	2.468	0.000	0.874	0.467
21–30	93	1.423	3.892	2.618	0.326	0.882	0.613
31–50	71	1.426	4.407	2.443	0.455	0.815	0.696
51–82	160	1.864	3.832	2.522	0.532	0.778	0.663
85–110	120	2.178	3.150	2.515	0.578	0.748	0.660
111–146	226	2.328	3.542	2.830	0.560	0.735	0.655
151–190	152	2.623	3.364	2.909	0.591	0.718	0.646
195–256	94	2.753	3.208	3.019	0.587	0.700	0.650
271–346	17	3.239	3.505	3.414	0.606	0.666	0.642

Both tables show, that the average path length is short with respect to n, whereas the clustering coefficient is high for most graph classes. Only the first graph class in each table has a small clustering coefficient, which is due to the small number of vertices in these graphs. Therefore networks with a number of vertices equal to or less than 10 were not considered for further evaluations. But as the other PPIN show the characteristics of small-world networks, small-world models were created for them.

Because the protein-protein interaction networks are undirected, the models were constructed after Watts and Strogatz with the additional probability q (see Section 2.3.3). For an extended Watts-Strogatz-Model the number of vertices n as well as the three parameters k, p and q are needed. The value for n was set to the number of vertices in the given PPIN and k, p as well as q were varied to find the best fitting values. For the

rewiring probability p the following values were used:

$$p \in \{0.01, 0.03, 0.05, 0.07, 0.1\}$$

The probability q for removing an edge was set to one of these five values:

$$q \in \{0, 0.3, 0.5, 0.7, 1\}$$

The range of the number of neighbours, k, was chosen according to the number of vertices. As a result of the remark in 2.3.1, the minimum number of neighbours is 4. The maximum number of neighbours, k_{max}, for networks in depth-full is defined as follows:

$$k_{max}^{(full)} = \begin{cases} \frac{n}{4} - \left(\frac{n}{4} \mod 2\right), & \text{if } n \leq 35 \\ 30, & \text{else} \end{cases}$$

For PPIN created with a depth of five, the maximum number of neighbours is:

$$k_{max}^{(5)} = \begin{cases} \frac{n}{2} - \left(\frac{n}{2} \mod 2\right), & \text{if } n \leq 50 \\ 30, & \text{else} \end{cases}$$

The values for k were then the set containing the numbers from 4 to k_{max} in steps of 2, which means:

$$k \in \{4, 6, ..., k_{max}\}$$

For each PPIN except those with $n \leq 10$ and every possible combination of k, p and q five models were created to avoid random effects and for each model, a quality measure similar to (3.2) was calculated. But since it is not possible to find a correct assignment between the vertices of the original PPIN and these from the model, QM_{deg} cannot be used. Instead the difference in the vertex distribution between model and original network, named QM_{vd}, is utilized. The quality measure for small-world models, $QM^{(SW)}$, is therefore:

$$\begin{aligned} QM^{(SW)} &= QM_{vd} + QM_m \\ &= \|deg_v(orig) - deg_v(model)\|_1 + |m(orig) - m(model)| \end{aligned} \tag{3.3}$$

with $deg_v(orig), deg_v(model)$ the vector of all vertex-degrees in ascending order for the original PPIN and the model, respectively, and $\|\cdot\|_1$ the Manhattan norm[11].
For each network and given q, parameters k and p of the model with the lowest quality measure were stored. The best k-p-combination of all PPIN is then the pair (k, p), which occurs most frequently.
Table 3.5 displays the averaged values of the quality measure $QM^{(SW)}$ for each graph class. This table shows, that the extended Watts-Strogatz-Model with probability $q = 0.7$ gets most frequently the best results followed by the model according to Newman and

[11] The Manhattan norm $\|\cdot\|_1$ for a d-dimensional vector x is defined as $\|x\|_1 = \sum_{i=1}^{d} |x_i|$

Watts. On the contrary, the original Watts-Strogatz-Model has never the lowest quality value, but in most cases the highest value for $QM^{(SW)}$.

Table 3.5: Averaged values of $QM^{(SW)}$ according to probability q

	range of n \ q	0	0.3	0.5	0.7	1
depth-full	16–35	50.62	53.62	54.62	55.14	57.62
	885–908	6953.49	6881.27	6810.3	6766.43	6849.96
depth-5	11–20	34	33.56	33.72	33.58	34.14
	21–30	89.65	89.89	89.08	89.92	89.76
	31–50	170.94	169.72	169.93	171.27	171.37
	51–82	389.98	391.81	391.11	391.15	391.09
	85–110	700.01	702.56	702.62	697.79	700.99
	111–146	922.4	922.89	918.59	913.15	918.7
	151–190	1162.97	1156.45	1154.08	1160.86	1184.42
	195–256	1633.53	1627.49	1618.89	1615.81	1642.55
	271–346	2243.88	2244.88	2263.88	2256	2252.12

Figure 3.4 shows the ratio between both differences of $QM^{(SW)}$. This diagram displays, that the differences in the vertex distribution have the major part of the quality measure, whereas the difference between the number of edges is more or less negligible, especially for huge graphs with $n \geq 50$.

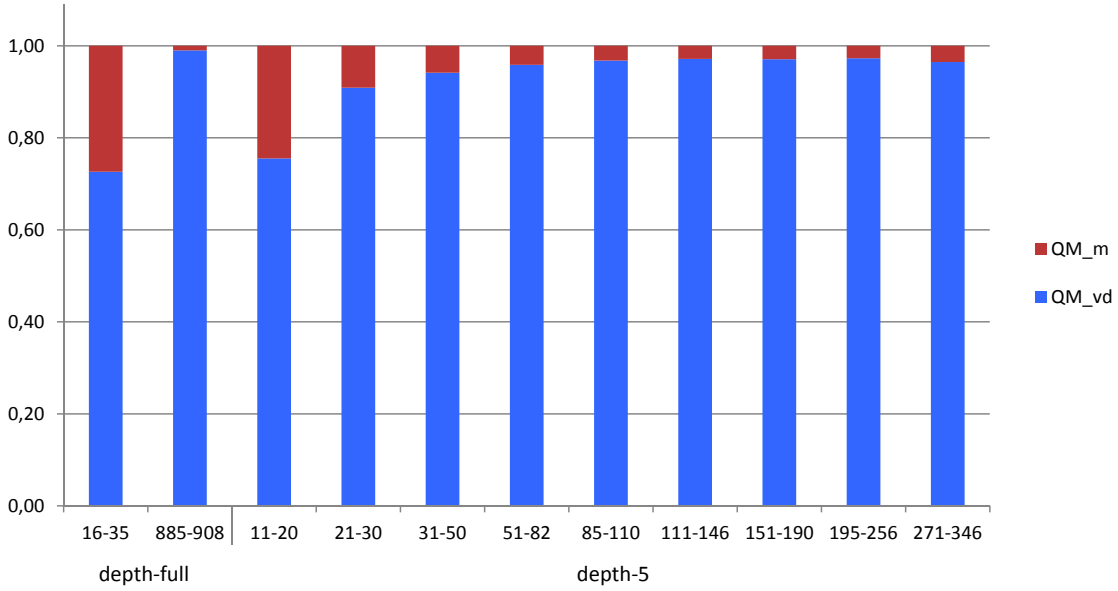


Figure 3.4: Partition of $QM^{(SW)}$

The best k-p-combinations for each graph class are shown in Table 3.6 and Table 3.7 for PPIN with full depth and depth-5, respectively. The entries in each row count, how

often this k-p-combination was the best one for all five values of q. A hyphen means, that this combination did not appear for the corresponding range of n. The results in these tables show, that for small graphs, which means $n \leq 35$ for depth-full and $n \leq 20$ for depth-5, $p = 0.01$ produces the best models and for huge networks, $p = 0.1$ yields the best fitting graphs. The number of neighbours must be chosen according to n, too. For graphs with $n \leq 35$, $k = 4$ produces good results and for bigger networks, k should be set to 10 for depth-full and to 12 or 14 for depth-5.

Table 3.6: Number of k-p-combinations for small-world models for depth-full

range of n \ (k,p)	$(4,0.01)$	$(10,0.05)$	$(10,0.1)$
16–35	5	-	-
885–908	-	2	3

Table 3.7: Number of k-p-combinations for small-world models for depth-5

range of n \ (k,p)	$(4,0.01)$	$(4,0.1)$	$(8,0.1)$	$(12,0.1)$	$(14,0.1)$	$(16,0.1)$
11–20	5	-	-	-	-	-
21–30	-	4	-	1	-	-
31–50	-	2	3	-	-	-
51–82	-	-	-	3	2	-
85–110	-	-	-	-	4	1
111–146	-	-	-	4	1	-
151–190	-	-	-	1	-	4
195–256	-	-	-	-	4	1
271–346	-	-	-	3	2	-

3.4 Comparison

The comparison between Exponential Random Graph Models and small-world models as well as the comparison with the Simple Random Graph Models from Erdős-Rényi and Gilbert are also made with the help of a quality measure. As already mentioned, the quality measure of ERGM is not suitable for small-world models. Furthermore it is not applicable for Erdős-Rényi- and Gilbert-Models, either. Therefore the quality measure of small-world models, $QM^{(SW)}$ (see (3.3)), is used.

To create an Erdős-Rényi- or a Gilbert-Model, the number of vertices is needed, which was set to the number of vertices in the original PPIN. Additionally, each model needs a second parameter: the number of edges m for the Erdős-Rényi-Model and the probability p that an edge exists for the Gilbert-Model. These two parameters were varied to

find the best fitting values. For this, 10 different Erdős-Rényi-Models should be created for each PPIN using different values for m. To accomplish this, the number of possible edges, which is $\binom{n}{2}$, was multiplied with $\frac{1}{10}, \frac{2}{10}, ..., \frac{10}{10}$ producing 10 evenly distributed values for m. The value for p was set to $0.2, 0.4, 0.6$ or 0.8 consecutively. For each PPIN and each parameter, 5 models were created to lessen random effects. The quality score for the model with the best parameter was stored and all these values were averaged. The results are listed in Table 3.8 and show, that the models after Erdős and Rényi are much better than the Gilbert-Models for the chosen parameter.

Table 3.8: Averaged values of $QM^{(SW)}$ for Erdős-Rényi- and Gilbert-Model

Model	Erdős-Rényi-Model	Gilbert-Model
depth-full	53759.31	114313.13
depth-5	725.43	2190.37

To compare all four models, the same test set of PPIN must be considered. Because the Exponential Random Graph Models were created only for some graphs from depth-5 and there were no small-world models constructed for graphs with $n \leq 10$, the test set contains only 234 remaining graphs from depth-5. The averaged values of the quality measure for each type of model can be found in Table 3.9. For Watts-Strogatz-Models representing the small-world models, the best value for the quality measure was chosen, which was gained with $q = 0.7$. It can be seen, that the Erdős-Rényi-Models have the lowest value for $QM^{(SW)}$, but the Watts-Strogatz-Models are almost on par. The Exponential Random Graph Models and the Gilbert-Models have a high quality value, which means, that they are not as suited for PPIN as the other two models. But ERGM could possibly produce better results, if other parameters than the chosen ones (number of edges, number of triangles, vertex-degree) are considered, for example the number of k-stars or the number of paths with a given length.

Table 3.9: Averaged values of $QM^{(SW)}$ for all four models

Model	Erdős-Rényi-Model	Gilbert-Model	ERGM	Watts-Strogatz-Model
$QM^{(SW)}$	884.35	2454.25	2254.69	979.79

The last comparison was done between the two Simple Random Graph Models and the small-world models. The graphs used for calculating the quality measure where those from depth-full and depth-5, which have a number of vertices greater than 10. The results are listed in Table 3.10. Again, for small-world models the Watts-Strogatz-Model with best quality score was chosen, which was received with $q = 0.7$. This table displays, that, especially for graphs from depth-full, the extended Watts-Strogatz-Models produce the best fitting models for PPIN.

Table 3.10: Averaged values of $QM^{(SW)}$ for Erdős-Rényi-, Gilbert- and Watts-Strogatz-Model

Model	Erdős-Rényi-Model	Gilbert-Model	Watts-Strogatz-Model
depth-full	85476.77	181757.22	5357.06
depth-5	828.53	2502.05	739.33

The comparisons mentioned above show, that neither ERGM with the three chosen parameters (see 3.2) nor the Gilbert-Model produce appropriate models for the protein-protein interaction network of E. coli. The best results were gained with the extended Watts-Strogatz-Model with $q = 0.7$ and the Erdős-Rényi-Model. The advantage of Erdős-Rényi-Models over Watts-Strogatz-Models is, that just two parameters, n and m, must be set, whereas for extended Watts-Strogatz-Models four parameters, n, k, p and q, have to be chosen. But the results in Section 3.3 show, that the choice for these parameters can be restricted to $q = 0.7$ as well as $k = 4$ and $p = 0.01$ for small graphs and $k = 10, 12$ or 14 and $p = 0.1$ for huge graphs, which simplifies the search for the best parameters significantly. Furthermore, as it can be seen in Table 3.10, the small-world models are much better than Erdős-Rényi-Models for graphs with a high number of vertices. Therefore, the extended Watts-Strogatz-Models produce the best fitting models for PPIN of E. coli.

4 Summary and Outlook

This master thesis dealt with Random Graph Models and their application to biological networks with the purpose to analyse the fitting of those models to graphs motivated by biological problems. For this, several Random Graph Models were considered and explained, for example common models as the Erdős-Rényi-Model and the Gilbert-Model. Furthermore, three more models were elaborated, namely the p_1-Model and its generalization the Exponential Random Graph Models as well as various models for the small-world problem, e.g. models suggested by Jon Kleinberg, Duncan Watts, Steven Strogatz or Mark Newman. Additionally, a new combination of Watts-Strogatz-Models and models from Newman and Watts was presented.
Thereon, four of the described models, Erdős-Rényi-Model, Gilbert-Model, ERGM with the explanatory variables number of edges, number of triangles and vertex-degree as well as extended Watts-Strogatz-Model, were tested with respect to the fitting to the protein-protein interaction network of the bacterium Escherichia coli. Thereto, different graphs were constructed with the help of those models and evaluated with a quality measure afterwards. The results showed, that the Gilbert-Model as well as the chosen Exponential Random Graph Model were not suitable for the PPIN of E. coli, whereas Erdős-Rényi-Model and extended Watts-Strogatz-Model produced good models. It is possible, that the ERGM can lead to better results if other explanatory variables than the chosen ones are used to create a random graph. For example, the influence of the number of k-stars, k-cycles or paths with length k on the fitting could be analysed. Furthermore, the conclusions made in this chapter indicate, that the new extended Watts-Strogatz-Model is better for the examined cases than the original models suggested by Watts, Strogatz and Newman and better than the Erdős-Rényi-Model, too.

In addition to the above mentioned ideas for further investigations on ERGM, other models can be examined, e.g. scale-free or preferential attachment models [1,2,25] as well as other small-world models. Furthermore, the comparison of the models in this thesis was restricted to undirected graphs because the chosen example of biological networks was based on undirected graphs. Thus, another comparison between those models should be executed for directed networks as well as for other biological networks than PPIN.

Appendix A: Exponential Random Graph Models

A.1 Output of R

```
R version 2.15.1 (2012-06-22) -- "Roasted Marshmallows"
Copyright (C) 2012 The R Foundation for Statistical Computing
ISBN 3-900051-07-0
Platform: x86_64-pc-mingw32/x64 (64-bit)

R ist freie Software und kommt OHNE JEGLICHE GARANTIE.

%Load needed library
> library("statnet")
Lade nötiges Paket: network
network: Classes for Relational Data
Version 1.7-1 created on March 1, 2012.
copyright (c) 2005, Carter T. Butts, University of California-Irvine
                    Mark S. Handcock, University of Washington
                    David R. Hunter, Penn State University
                    Martina Morris, University of Washington

Lade nötiges Paket: ergm
Lade nötiges Paket: robustbase
Lade nötiges Paket: Matrix
Lade nötiges Paket: lattice
Lade nötiges Paket: trust
Lade nötiges Paket: nlme
Lade nötiges Paket: coda
ergm: version 3.0-3, created on 2012-05-27
Copyright (c) 2003, Mark S. Handcock, University of California-Los Angeles
                    David R. Hunter, Penn State University
                    Carter T. Butts, University of California-Irvine
                    Steven M. Goodreau, University of Washington
                    Pavel N. Krivitsky, Penn State University
                    Martina Morris, University of Washington
Based on "statnet" project software (statnet.org).

%Define a network from a matrix
> m <- matrix(c(0,1,0,0,1,1,0,0,0,1,0,0,0,1,1,0,0,1,0,1,1,1,1,1,0),
ncol=5, nrow=5, byrow=TRUE)
> n <- network(m, directed=FALSE)
```

```
%Display the network
> n
 Network attributes:
  vertices = 5
  directed = FALSE
  hyper = FALSE
  loops = FALSE
  multiple = FALSE
  bipartite = FALSE
  total edges= 6
    missing edges= 0
    non-missing edges= 6

 Vertex attribute names:
    vertex.names

%Execute ERGM with given explanatory variables
> results <- ergm(n ~ edges + triangles + sociality(base=0))
Observed statistic(s) sociality5 are at their greatest attainable values.
Their coefficients will be fixed at +Inf.
Iteration 1 of at most 20:
the log-likelihood improved by 0.02527
Iteration 2 of at most 20:
the log-likelihood improved by 0.01282
Iteration 3 of at most 20:
the log-likelihood improved by 0.007614
Iteration 4 of at most 20:
the log-likelihood improved by 0.004278
Iteration 5 of at most 20:
the log-likelihood improved by 0.002748
Iteration 6 of at most 20:
the log-likelihood improved by 0.001508
Iteration 7 of at most 20:
the log-likelihood improved by 0.001313
Iteration 8 of at most 20:
the log-likelihood improved by 0.0005915
Iteration 9 of at most 20:
the log-likelihood improved by 0.0003724
Iteration 10 of at most 20:
the log-likelihood improved by 0.0001881
Iteration 11 of at most 20:
the log-likelihood improved by 0.0001625
Iteration 12 of at most 20:
the log-likelihood improved by 0.0002098
Iteration 13 of at most 20:
the log-likelihood improved by 0.0001119
```

```
Iteration 14 of at most 20:
Convergence detected. Stopping early.
the log-likelihood improved by < 0.0001

This model was fit using MCMC.  To examine model diagnostics and
check for degeneracy, use the mcmc.diagnostics() function.

%Display the results
> summary(results)

==========================
Summary of model fit
==========================

Formula:   n ~ edges + triangles + sociality(base = 0)
Iterations:  20

Monte Carlo MLE Results:
             Estimate Std. Error MCMC % p-value
edges       4.111e+00  6.740e+06     NA   1.000
triangle   -7.367e+00  1.284e+02     NA   0.958
sociality1  1.434e+00  3.370e+06     NA   1.000
sociality2  1.432e+00  3.370e+06     NA   1.000
sociality3  1.434e+00  3.370e+06     NA   1.000
sociality4  1.432e+00  3.370e+06     NA   1.000
sociality5        Inf         NA     NA      NA

Warning:  The standard errors are suspect due to possible poor convergence.

    Null  Deviance: 13.863  on 10  degrees of freedom
 Residual Deviance:    NaN  on  3  degrees of freedom
          Deviance:    NaN  on  7  degrees of freedom

AIC: NaN    BIC: NaN

 Warning: The following terms have infinite coefficient estimates:
  sociality5
```

A.2 Results for ERGM

This table shows the lowest (**min**) and the highest (**max**) value for each explanatory variable (**parameter**) of the ERGM (3.1) as well as the number of values (**num**), which were computed through "statnet". Additionally, the average values (**avg**) for each of these parameters is given. If an explanatory variable had one or more values equal to $\pm\infty$, the value was set to ± 1000 to get a valid average. Furthermore the average over all values unequal to $\pm\infty$ was calculated (**avg$_{\text{no inf}}$**). A hyphen means, that for this explanatory variable no average without values equal to $\pm\infty$ could be calculated, because all values computed by "statnet" were equal to $\pm\infty$.

Table A.1: Results for the explanatory variables of ERGM (3.1)

parameter	θ	ρ	α_{0002}	α_{0003}	α_{0004}	α_{0008}	α_{0025}
num	913	913	265	195	98	237	9
min	-78,08	-∞	-3,03	-1,7	-1,7	-7,28	-0,42
max	∞	49,13	2,19	3,29	2,46	1,92	0,23
avg	3,08	-94,87	-0,81	0,39	1,06	-0,86	0,09
avg$_{\text{no inf}}$	1,99	0,46	-0,81	0,39	1,06	-0,86	0,09
parameter	α_{0026}	α_{0029}	α_{0030}	α_{0031}	α_{0032}	α_{0033}	α_{0036}
num	16	17	62	62	169	169	4
min	-47,13	-47,13	-47,13	-1,34	-2,54	-2,55	∞
max	1,2	1,38	1,98	3,06	2,43	2,42	∞
avg	-2,9	-2,89	-3,93	0,58	-0,33	-0,33	∞
avg$_{\text{no inf}}$	-2,9	-2,89	-3,93	0,58	-0,33	-0,33	-
parameter	α_{0037}	α_{0038}	α_{0039}	α_{0048}	α_{0052}	α_{0061}	α_{0062}
num	4	3	3	245	74	49	13
min	-47,13	-47,13	-47,13	-3,89	-1,01	-47,13	-47,13
max	-47,13	0	0	2,05	1,52	3,66	-0,41
avg	-47,13	-15,71	-15,71	0,33	0,44	-0,36	-4,79
avg$_{\text{no inf}}$	-47,13	-15,71	-15,71	0,33	0,44	-0,36	-4,79
parameter	α_{0063}	α_{0071}	α_{0072}	α_{0073}	α_{0074}	α_{0077}	α_{0078}
num	45	247	247	89	297	247	247
min	-1,02	-5,68	-5,67	-0,66	-47,13	-5,73	-5,73
max	∞	7,35	7,34	6,35	8,1	8,09	8,1
avg	23,29	-2,37	-2,37	0,85	-1,61	-2,15	-2,15
avg$_{\text{no inf}}$	1,09	-2,37	-2,37	0,85	-1,61	-2,15	-2,15
parameter	α_{0084}	α_{0085}	α_{0086}	α_{0087}	α_{0088}	α_{0090}	α_{0091}
num	20	59	48	28	84	22	37
min	-4,08	-3,8	-10,81	-51,13	-3,72	-1,38	-1,74
max	1,33	2,12	1,22	0,39	3,5	∞	2,14
avg	0	-0,25	-0,76	-2,39	0,18	46,59	-0,31
avg$_{\text{no inf}}$	0	-0,25	-0,76	-2,39	0,18	1,19	-0,31

parameter	α_{0092}	α_{0096}	α_{0103}	α_{0104}	α_{0109}	α_{0114}	α_{0115}
num	28	32	4	108	32	315	277
min	-3,25	-2,83	-1,51	-2,3	-0,32	-4,12	-2,44
max	0,55	0,93	-0,74	1,1	1,23	8,33	1,45
avg	-0,37	-0,47	-1,04	-0,71	0,16	-1	-0,84
avg$_{\text{no inf}}$	-0,37	-0,47	-1,04	-0,71	0,16	-1	-0,84
parameter	α_{0116}	α_{0118}	α_{0120}	α_{0121}	α_{0124}	α_{0125}	α_{0126}
num	291	126	92	93	219	106	9
min	-3,75	-0,82	-1,5	-1,28	-5,65	-1,19	-0,23
max	2,39	2,19	1,6	2,52	2,12	1,63	1,3
avg	0,26	0,41	-0,31	0,31	-0,26	-0,06	0,01
avg$_{\text{no inf}}$	0,26	0,41	-0,31	0,31	-0,26	-0,06	0,01
parameter	α_{0129}	α_{0131}	α_{0133}	α_{0134}	α_{0142}	α_{0149}	α_{0150}
num	56	241	119	36	31	19	8
min	-3,63	-3,12	-1,46	-1,54	-1,6	-7,14	-42,61
max	1,7	1,01	2,35	2,47	1,06	0	-19,93
avg	-0,29	-1,29	0,83	1,04	-0,61	-1,51	-26
avg$_{\text{no inf}}$	-0,29	-1,29	0,83	1,04	-0,61	-1,51	-26
parameter	α_{0151}	α_{0152}	α_{0153}	α_{0154}	α_{0158}	α_{0159}	α_{0160}
num	8	8	8	5	5	61	81
min	-35,37	-35,37	-37,39	-1,72	-66,27	-1,14	-0,5
max	-19,04	-19,04	-19,31	-0,01	-20,09	1,15	1,31
avg	-21,82	-21,82	-23	-0,74	-29,46	-0,35	0,24
avg$_{\text{no inf}}$	-21,82	-21,82	-23	-0,74	-29,46	-0,35	0,24
parameter	α_{0166}	α_{0167}	α_{0171}	α_{0173}	α_{0174}	α_{0175}	α_{0179}
num	56	5	39	14	12	49	28
min	-1,34	-0,61	-1,56	-25,16	-47,13	-1,69	-1,87
max	0,88	∞	1,18	0,99	-1,07	1,6	1,89
avg	-0,15	200,09	-0,26	-2,94	-5,38	0,34	0,36
avg$_{\text{no inf}}$	-0,15	0,12	-0,26	-2,94	-5,38	0,34	0,36
parameter	α_{0180}	α_{0181}	α_{0182}	α_{0184}	α_{0185}	α_{0186}	α_{0196}
num	9	32	27	76	193	47	4
min	-1,91	-1,55	-2,5	-1,57	-3,21	-1,48	-47,13
max	0,87	1,12	1,89	0,27	1,24	1,15	2,12
avg	-0,27	-0,02	0,18	-0,58	-1,35	-0,82	-11,05
avg$_{\text{no inf}}$	-0,27	-0,02	0,18	-0,58	-1,35	-0,82	-11,05

parameter	α_{0207}	α_{0212}	α_{0215}	α_{0221}	α_{0237}	α_{0238}	α_{0242}
num	9	11	76	50	264	80	248
min	-5,23	-0,86	-1,57	-0,37	-3,55	-1,25	-4,3
max	1,2	5,37	0,26	2,2	1,1	1,69	0,04
avg	-1,37	0,45	-0,58	0,63	-1,45	-0,04	-2,46
avg$_{\text{no inf}}$	-1,37	0,45	-0,58	0,63	-1,45	-0,04	-2,46
parameter	α_{0243}	α_{0261}	α_{0268}	α_{0269}	α_{0271}	α_{0273}	α_{0284}
num	76	160	100	62	42	123	69
min	-1,07	-2,22	-0,91	-0,65	-47,13	-1,66	-1,03
max	2,74	2,61	3,08	2,28	0,15	3,02	1,45
avg	0,12	-0,09	0,3	0,74	-2,07	0,17	0,17
avg$_{\text{no inf}}$	0,12	-0,09	0,3	0,74	-2,07	0,17	0,17
parameter	α_{0285}	α_{0286}	α_{0311}	α_{0312}	α_{0323}	α_{0331}	α_{0333}
num	69	69	25	7	240	89	95
min	-1,04	-1,04	-0,13	-47,13	-3,03	-1,19	-0,78
max	1,45	1,45	∞	-1,27	0,92	1,64	1,76
avg	0,17	0,17	119,98	-20,95	-1,49	-0,1	0,12
avg$_{\text{no inf}}$	0,17	0,17	-0,02	-20,95	-1,49	-0,1	0,12
parameter	α_{0334}	α_{0335}	α_{0337}	α_{0339}	α_{0340}	α_{0344}	α_{0347}
num	87	87	22	9	43	69	4
min	-1,58	-0,78	-0,03	-0,24	-0,27	-47,13	-4,06
max	1,38	1,76	1,39	1,3	2,2	1,51	0,84
avg	-0,32	0	0,7	0	0,27	-0,64	-1,14
avg$_{\text{no inf}}$	-0,32	0	0,7	0	0,27	-0,64	-1,14
parameter	α_{0348}	α_{0349}	α_{0350}	α_{0351}	α_{0352}	α_{0355}	α_{0356}
num	5	5	10	190	36	34	20
min	-1,34	-6,37	-2,01	-5,09	-1,13	-0,98	-1,84
max	16,31	0,86	0,84	1	0,84	1,3	0,63
avg	3,52	-1,23	-0,76	-1,35	-0,5	-0,07	-0,41
avg$_{\text{no inf}}$	3,52	-1,23	-0,76	-1,35	-0,5	-0,07	-0,41
parameter	α_{0368}	α_{0369}	α_{0381}	α_{0383}	α_{0386}	α_{0388}	α_{0394}
num	79	5	29	16	22	8	143
min	-0,67	-6,72	-3,25	-0,97	-1,42	-37,5	-4,01
max	2,9	-0,01	0,55	1,15	1,75	0,75	2,18
avg	0,18	-1,79	-0,37	-0,24	-0,18	-6,85	-0,22
avg$_{\text{no inf}}$	0,18	-1,79	-0,37	-0,24	-0,18	-6,85	-0,22

parameter	α_{0403}	α_{0404}	α_{0414}	α_{0415}	α_{0417}	α_{0418}	α_{0420}
num	35	43	64	38	58	12	15
min	-1,52	-0,86	-2,2	-1,79	-2,14	-4,14	-23,33
max	0,7	1,83	0,72	1,37	1,94	0,14	0,67
avg	-0,22	0,55	-0,31	0,02	0,13	-1,1	-2,68
$\text{avg}_{\text{no inf}}$	-0,22	0,55	-0,31	0,02	0,13	-1,1	-2,68
parameter	α_{0421}	α_{0423}	α_{0425}	α_{0428}	α_{0429}	α_{0430}	α_{0431}
num	18	13	44	51	88	88	88
min	-3,35	-0,43	-1,4	-3,97	-35,27	-35,27	-35,27
max	∞	2,15	1,14	14,47	0,5	0,51	0,5
avg	55,46	0,12	0,2	0,05	-1,92	-1,92	-1,92
$\text{avg}_{\text{no inf}}$	-0,1	0,12	0,2	0,05	-1,92	-1,92	-1,92
parameter	α_{0432}	α_{0450}	α_{0462}	α_{0463}	α_{0469}	α_{0470}	α_{0474}
num	88	5	8	8	143	76	141
min	-35,27	-47,13	-1,18	0	-4	-1,61	-47,13
max	0,51	0,34	0	0,85	∞	0,27	2,12
avg	-1,92	-9,63	-0,59	0,43	35,16	-0,58	-0,27
$\text{avg}_{\text{no inf}}$	-1,92	-9,63	-0,59	0,43	0,2	-0,58	-0,27
parameter	α_{0475}	α_{0477}	α_{0480}	α_{0485}	α_{0494}	α_{0507}	α_{0508}
num	47	108	145	267	6	107	43
min	-2,4	-2,18	-5,36	-3,06	-2,22	-2,42	-0,77
max	73,65	1,1	1,93	1,36	-0,21	1,66	1,57
avg	3,36	-0,56	0,29	-1,18	-1,15	0,04	0,01
$\text{avg}_{\text{no inf}}$	3,36	-0,56	0,29	-1,18	-1,15	0,04	0,01
parameter	α_{0509}	α_{0514}	α_{0521}	α_{0522}	α_{0523}	α_{0524}	α_{0529}
num	44	40	240	31	43	25	221
min	-0,55	-0,92	-3,03	-1,09	-1,91	-2,49	-3,42
max	1,96	1,8	0,91	0,28	0,3	0,93	2,03
avg	0,22	0,02	-1,49	-0,44	-0,32	-0,3	0,35
$\text{avg}_{\text{no inf}}$	0,22	0,02	-1,49	-0,44	-0,32	-0,3	0,35
parameter	α_{0583}	α_{0584}	α_{0586}	α_{0588}	α_{0589}	α_{0590}	α_{0591}
num	18	8	18	8	8	8	4
min	-1,52	-41,29	-1,54	-35,36	-36,27	-36,3	-15,92
max	1,1	-19,79	1,1	-19,03	-19,17	-19,16	-15,92
avg	0,36	-25,23	0,36	-21,82	-22,37	-22,37	-15,92
$\text{avg}_{\text{no inf}}$	0,36	-25,23	0,36	-21,82	-22,37	-22,37	-15,92

parameter	α_{0592}	α_{0593}	α_{0594}	α_{0595}	α_{0596}	α_{0612}	α_{0613}
num	8	145	18	52	20	68	68
min	-35,37	-4,06	-1,52	-2,96	-1,48	-0,47	-0,48
max	-19,02	2,86	1,1	1,38	1,54	1,76	1,75
avg	-21,81	0,31	0,36	-0,17	0,56	0,3	0,3
avg$_{\text{no inf}}$	-21,81	0,31	0,36	-0,17	0,56	0,3	0,3
parameter	α_{0614}	α_{0615}	α_{0616}	α_{0617}	α_{0618}	α_{0632}	α_{0635}
num	68	217	218	217	68	18	18
min	-0,48	-6,28	-6,29	-6,28	-0,48	-10,77	-10,76
max	1,75	2,13	2,16	2,15	1,76	-0,92	-0,92
avg	0,3	0,02	0,02	0,02	0,3	-2,3	-2,3
avg$_{\text{no inf}}$	0,3	0,02	0,02	0,02	0,3	-2,3	-2,3
parameter	α_{0638}	α_{0639}	α_{0640}	α_{0642}	α_{0662}	α_{0674}	α_{0677}
num	1	38	76	15	12	296	76
min	∞	-0,33	-1,61	-1,76	-3,37	-5,17	-2,27
max	∞	3,24	0,27	1,2	0,07	1,36	1,5
avg	∞	0,32	-0,58	0,05	-0,9	-1,1	-0,06
avg$_{\text{no inf}}$	-	0,32	-0,58	0,05	-0,9	-1,1	-0,06
parameter	α_{0678}	α_{0679}	α_{0688}	α_{0693}	α_{0720}	α_{0721}	α_{0722}
num	79	93	239	73	331	189	189
min	-1,86	-3,31	-5,15	-2,83	-6,28	-74,58	-74,58
max	1,22	1,81	1,64	2,2	2,16	1,57	1,58
avg	-0,52	-0,19	-0,67	0,29	-0,55	-0,64	-0,64
avg$_{\text{no inf}}$	-0,52	-0,19	-0,67	0,29	-0,55	-0,64	-0,64
parameter	α_{0723}	α_{0724}	α_{0726}	α_{0727}	α_{0728}	α_{0729}	α_{0731}
num	189	189	214	130	149	149	58
min	-74,58	-74,58	-2,77	-0,42	-0,48	-0,49	-3,32
max	1,57	1,57	2,53	2,21	2,44	2,44	1,83
avg	-0,64	-0,64	0,25	0,68	0,71	0,71	-0,45
avg$_{\text{no inf}}$	-0,64	-0,64	0,25	0,68	0,71	0,71	-0,45
parameter	α_{0732}	α_{0733}	α_{0734}	α_{0736}	α_{0750}	α_{0754}	α_{0755}
num	8	55	55	15	35	4	198
min	-1,61	-3,52	-3,51	-2,21	-1,04	-47,13	-4,7
max	0,7	-0,23	-0,23	0,34	1,12	-2,89	1,34
avg	-0,59	-2,02	-2,02	-0,98	-0,11	-28,81	-1,67
avg$_{\text{no inf}}$	-0,59	-2,02	-2,02	-0,98	-0,11	-28,81	-1,67

parameter	α_{0756}	α_{0757}	α_{0758}	α_{0759}	α_{0766}	α_{0767}	α_{0771}
num	58	78	161	64	142	37	113
min	-0,94	-1,15	-3,71	-4,61	-2,3	-1,46	-0,97
max	1,07	1,72	2,17	1,7	1,52	0,45	1,71
avg	-0,44	-0,04	0,07	-0,56	-0,5	-0,05	0,1
$\text{avg}_{\text{no inf}}$	-0,44	-0,04	0,07	-0,56	-0,5	-0,05	0,1
parameter	α_{0774}	α_{0775}	α_{0776}	α_{0777}	α_{0778}	α_{0789}	α_{0823}
num	10	6	11	18	7	43	319
min	-2,34	-17,97	-48,34	-2,34	-1,34	-0,74	-4,45
max	47,77	0,46	23,39	0,74	23,39	1,79	7,68
avg	6,22	-3,37	-2,04	0,12	3,66	0,3	-0,51
$\text{avg}_{\text{no inf}}$	6,22	-3,37	-2,04	0,12	3,66	0,3	-0,51
parameter	α_{0839}	α_{0841}	α_{0870}	α_{0871}	α_{0878}	α_{0879}	α_{0893}
num	18	21	128	247	4	4	8
min	-10,8	-3,16	-0,3	-4,18	-0,03	-0,03	-47,13
max	-0,92	-0,01	2,54	8,08	-0,03	-0,03	-0,08
avg	-2,3	-0,9	0,83	-1,56	-0,03	-0,03	-6,14
$\text{avg}_{\text{no inf}}$	-2,3	-0,9	0,83	-1,56	-0,03	-0,03	-6,14
parameter	α_{0894}	α_{0895}	α_{0896}	α_{0903}	α_{0907}	α_{0908}	α_{0910}
num	34	34	34	319	77	9	53
min	-3,64	-3,65	-3,63	-4,45	-0,57	-39,22	-0,99
max	0,38	0,4	0,36	7,66	1,94	1,01	1,18
avg	-0,29	-0,29	-0,29	-0,51	0,92	-6,85	-0,16
$\text{avg}_{\text{no inf}}$	-0,29	-0,29	-0,29	-0,51	0,92	-6,85	-0,16
parameter	α_{0915}	α_{0918}	α_{0928}	α_{0931}	α_{0932}	α_{0945}	α_{0954}
num	22	12	385	31	165	32	9
min	-1,98	-47,54	-3,99	-0,48	-1,24	-1,78	-1,84
max	0,93	3,84	2,42	0,55	2,73	0,21	1,69
avg	-0,47	-4,41	-0,58	-0,06	0,28	-1,04	0,29
$\text{avg}_{\text{no inf}}$	-0,47	-4,41	-0,58	-0,06	0,28	-1,04	0,29
parameter	α_{0963}	α_{0968}	α_{0978}	α_{0979}	α_{0980}	α_{0996}	α_{0997}
num	115	24	55	55	9	34	34
min	-1,47	-0,35	-3,53	-3,52	-0,42	-3,48	-3,44
max	5,63	1,12	-0,23	-0,23	0,23	0,52	0,52
avg	0,31	-0,21	-2,02	-2,02	0,09	-0,27	-0,27
$\text{avg}_{\text{no inf}}$	0,31	-0,21	-2,02	-2,02	0,09	-0,27	-0,27

parameter	α_{0998}	α_{1002}	α_{1008}	α_{1009}	α_{1010}	α_{1011}	α_{1012}
num	14	173	1	1	2	1	1
min	-0,44	-5,46	-47,13	∞	-47,13	∞	-47,13
max	-0,07	2,1	-47,13	∞	-47,13	∞	-47,13
avg	-0,41	-0,02	-47,13	∞	-47,13	∞	-47,13
avg$_{\text{no inf}}$	-0,41	-0,02	-47,13	-	-47,13	-	-47,13
parameter	α_{1014}	α_{1033}	α_{1054}	α_{1062}	α_{1090}	α_{1091}	α_{1092}
num	284	172	10	15	20	120	76
min	-3,61	-2,42	-1,7	-0,56	-0,89	-0,94	-2,07
max	3,77	2,89	0,4	0,2	3,2	2,46	2,34
avg	-1,96	0,43	-0,82	0,05	0,21	0,43	0,63
avg$_{\text{no inf}}$	-1,96	0,43	-0,82	0,05	0,21	0,43	0,63
parameter	α_{1093}	α_{1094}	α_{1095}	α_{1096}	α_{1098}	α_{1099}	α_{1101}
num	22	89	28	31	50	76	240
min	-1,14	-5,6	-1,73	-2,88	-0,63	-1,58	-6,25
max	3,03	2,19	3,03	1,42	1,18	0,28	1,15
avg	1,47	0,01	1,18	-1,08	0	-0,58	-1,82
avg$_{\text{no inf}}$	1,47	0,01	1,18	-1,08	0	-0,58	-1,82
parameter	α_{1106}	α_{1107}	α_{1119}	α_{1120}	α_{1131}	α_{1136}	α_{1189}
num	58	33	60	79	216	213	219
min	-2,14	-2,17	-1,94	-1,86	-47,13	-2,77	-3,55
max	1,94	1,32	1,63	1,24	1,9	2,6	1,82
avg	0,13	-0,24	0,03	-0,52	-0,11	0,36	-1,15
avg$_{\text{no inf}}$	0,13	-0,24	0,03	-0,52	-0,11	0,36	-1,15
parameter	α_{1190}	α_{1197}	α_{1198}	α_{1199}	α_{1200}	α_{1207}	α_{1208}
num	70	16	10	16	16	172	15
min	-3,86	-47,13	-4,11	-0,73	-0,73	-1,94	-4,29
max	2,03	-0,64	1,2	3,19	3,21	2,42	0,64
avg	-0,22	-16,01	-1,28	0,24	0,24	0,5	-0,75
avg$_{\text{no inf}}$	-0,22	-16,01	-1,28	0,24	0,24	0,5	-0,75
parameter	α_{1210}	α_{1215}	α_{1224}	α_{1225}	α_{1226}	α_{1227}	α_{1232}
num	29	5	34	34	17	34	251
min	-1,39	-1,03	-3,52	-3,49	0,44	-3,5	-5,06
max	2,12	∞	0,77	0,76	0,88	0,78	1,81
avg	-0,43	201,11	-0,11	-0,11	0,52	-0,11	-0,28
avg$_{\text{no inf}}$	-0,43	1,39	-0,11	-0,11	0,52	-0,11	-0,28

parameter	α_{1236}	α_{1238}	α_{1241}	α_{1249}	α_{1252}	α_{1260}	α_{1261}
num	161	37	189	43	8	137	137
min	-2,13	0,11	-5,09	-0,73	∞	-0,93	-0,91
max	2,28	1,37	0,78	1,78	∞	2,49	2,49
avg	0,42	0,46	-1,39	0,3	∞	0,22	0,22
avg$_{\text{no inf}}$	0,42	0,46	-1,39	0,3	-	0,22	0,22
parameter	α_{1262}	α_{1263}	α_{1264}	α_{1270}	α_{1276}	α_{1277}	α_{1278}
num	37	74	61	1	123	96	11
min	-1,49	-3,99	-3,99	-47,13	-0,82	-4,14	-4,14
max	1,43	1,84	1,68	-47,13	1,85	1,17	0,14
avg	-0,11	-0,06	-0,29	-47,13	0,2	-1,01	-1,15
avg$_{\text{no inf}}$	-0,11	-0,06	-0,29	-47,13	0,2	-1,01	-1,15
parameter	α_{1281}	α_{1288}	α_{1297}	α_{1298}	α_{1300}	α_{1301}	α_{1302}
num	65	11	252	271	30	15	155
min	-1,96	-3,04	-4,3	-4,16	-1,36	-2,05	-1,66
max	0,81	3,56	0,98	0,03	1,37	1,2	2,07
avg	-0,54	0,49	-2,2	-2,3	-0,62	-0,79	0,62
avg$_{\text{no inf}}$	-0,54	0,49	-2,2	-2,3	-0,62	-0,79	0,62
parameter	α_{1309}	α_{1380}	α_{1385}	α_{1386}	α_{1387}	α_{1388}	α_{1389}
num	154	247	9	79	20	8	8
min	-5,46	-4,6	-205,5	-3,27	-0,52	-0,37	-0,37
max	1,88	8,34	1,89	1,38	1,9	2,16	2,09
avg	-0,26	-1,81	-23,18	0,26	0,16	0,42	0,41
avg$_{\text{no inf}}$	-0,26	-1,81	-23,18	0,26	0,16	0,42	0,41
parameter	α_{1390}	α_{1392}	α_{1393}	α_{1394}	α_{1395}	α_{1397}	α_{1398}
num	8	8	19	22	32	18	8
min	-0,38	-0,38	-0,77	-51,08	-0,41	-0,6	-1,35
max	1,92	1,95	0,51	3,41	2,13	0,35	2,24
avg	0,38	0,39	0	-2,14	-0,04	-0,17	0,07
avg$_{\text{no inf}}$	0,38	0,39	0	-2,14	-0,04	-0,17	0,07
parameter	α_{1409}	α_{1415}	α_{1421}	α_{1444}	α_{1465}	α_{1466}	α_{1467}
num	45	323	14	244	34	3	34
min	-1,71	-4,6	-47,13	-3,72	-3,49	0,07	-3,53
max	1,6	9,34	0,98	0,61	0,69	0,07	0,67
avg	0,2	-0,89	-3,38	-1,8	-0,15	0,07	-0,16
avg$_{\text{no inf}}$	0,2	-0,89	-3,38	-1,8	-0,15	0,07	-0,16

parameter	α_{1468}	α_{1474}	α_{1475}	α_{1476}	α_{1478}	α_{1479}	α_{1493}
num	34	113	113	113	35	294	271
min	-3,49	-2,21	-2,22	-2,22	-1,03	-4,23	-4,02
max	0,69	1,39	1,39	1,39	1,02	7,86	0,24
avg	-0,15	-0,92	-0,92	-0,92	-0,09	-1,13	-2,07
avg$_{\text{no inf}}$	-0,15	-0,92	-0,92	-0,92	-0,09	-1,13	-2,07
parameter	α_{1501}	α_{1521}	α_{1524}	α_{1525}	α_{1584}	α_{1593}	α_{1602}
num	110	4	267	21	58	7	21
min	-1,98	-1,65	-3,06	-0,92	-1,56	-1,33	-0,2
max	1,1	-0,19	1,36	1,11	2,4	23,39	3,24
avg	-1,08	-1,22	-1,18	0,67	0,01	3,73	0,62
avg$_{\text{no inf}}$	-1,08	-1,22	-1,18	0,67	0,01	3,73	0,62
parameter	α_{1603}	α_{1606}	α_{1611}	α_{1612}	α_{1613}	α_{1617}	α_{1621}
num	21	245	159	159	140	1	229
min	-0,19	-3,89	-0,82	-0,84	-3,85	-1,3	-6,25
max	3,24	2,05	1,82	1,82	1,89	-1,3	1,16
avg	0,62	0,33	0,24	0,24	-0,44	-1,3	-1,96
avg$_{\text{no inf}}$	0,62	0,33	0,24	0,24	-0,44	-1,3	-1,96
parameter	α_{1622}	α_{1623}	α_{1635}	α_{1636}	α_{1638}	α_{1640}	α_{1646}
num	269	66	50	10	13	12	32
min	-4,18	-0,98	-0,79	-23,54	-22,13	-0,93	-0,96
max	1,89	1,18	3,27	0,07	0,71	-0,62	1,5
avg	-0,97	-0,09	0,4	-4,07	-2,52	-0,82	0,07
avg$_{\text{no inf}}$	-0,97	-0,09	0,4	-4,07	-2,52	-0,82	0,07
parameter	α_{1651}	α_{1656}	α_{1662}	α_{1676}	α_{1680}	α_{1692}	α_{1693}
num	128	32	37	324	23	4	5
min	-1,47	-0,96	-2,2	-4,07	-1,6	-36,5	-47,13
max	5,82	1,5	∞	7,87	1,44	1,02	0,09
avg	0,34	0,07	27	-0,76	0,04	-12,74	-19,98
avg$_{\text{no inf}}$	0,34	0,07	-0,03	-0,76	0,04	-12,74	-19,98
parameter	α_{1695}	α_{1701}	α_{1702}	α_{1704}	α_{1709}	α_{1710}	α_{1711}
num	6	19	247	3	4	50	4
min	-0,21	-1,77	-3,97	-41	-20,66	-1	-20,64
max	0,72	0,01	8,11	-2,88	-19,99	3,08	-19,98
avg	0,23	-0,99	-1,43	-22,83	-20,21	0,2	-20,17
avg$_{\text{no inf}}$	0,23	-0,99	-1,43	-22,83	-20,21	0,2	-20,17

parameter	α_{1723}	α_{1727}	α_{1732}	α_{1734}	α_{1736}	α_{1737}	α_{1738}
num	190	90	32	42	58	58	58
min	-3,81	-2,14	-0,29	-2,24	-3,31	-3,31	-3,31
max	2	2,83	2,17	0,91	1,64	1,64	1,64
avg	-0,49	0,36	0,76	-0,65	-0,2	-0,2	-0,19
$\text{avg}_{\text{no inf}}$	-0,49	0,36	0,76	-0,65	-0,2	-0,2	-0,19
parameter	α_{1740}	α_{1744}	α_{1745}	α_{1746}	α_{1747}	α_{1748}	α_{1761}
num	200	249	26	17	38	24	349
min	-3,54	-4,3	-0,95	-0,73	-1,66	-1,15	-3,75
max	1,82	0,04	0	1,57	0,47	0,95	0,91
avg	-1,75	-2,5	-0,66	-0,34	0,03	0,09	-1,57
$\text{avg}_{\text{no inf}}$	-1,75	-2,5	-0,66	-0,34	0,03	0,09	-1,57
parameter	α_{1764}	α_{1767}	α_{1768}	α_{1779}	α_{1780}	α_{1781}	α_{1800}
num	42	302	14	197	219	5	227
min	-47,13	-3,79	-0,52	-3,78	-5,15	-3,96	-2,64
max	1,39	1,36	0,8	1,47	1,2	0,43	6,47
avg	-0,96	-1,23	-0,27	-1,36	-1,93	-1,39	-0,31
$\text{avg}_{\text{no inf}}$	-0,96	-1,23	-0,27	-1,36	-1,93	-1,39	-0,31
parameter	α_{1805}	α_{1812}	α_{1814}	α_{1817}	α_{1818}	α_{1819}	α_{1842}
num	19	9	173	96	96	96	76
min	-1,75	-1,4	-2,86	-3,31	-3,31	-3,31	-1,58
max	0	1,09	2,76	1,87	1,88	1,88	0,25
avg	-0,99	-0,29	0,13	-0,24	-0,24	-0,24	-0,58
$\text{avg}_{\text{no inf}}$	-0,99	-0,29	0,13	-0,24	-0,24	-0,24	-0,58
parameter	α_{1849}	α_{1850}	α_{1851}	α_{1852}	α_{1854}	α_{1855}	α_{1865}
num	229	311	84	15	324	9	8
min	-3,18	-6,02	-1,22	-1,33	-4,07	-2,43	-1,07
max	2,55	2,55	1,47	0,29	7,87	1,4	0,01
avg	0,14	0,03	0,11	-0,68	-0,76	0,08	-0,75
$\text{avg}_{\text{no inf}}$	0,14	0,03	0,11	-0,68	-0,76	0,08	-0,75
parameter	α_{1872}	α_{1873}	α_{1881}	α_{1882}	α_{1883}	α_{1884}	α_{1885}
num	35	35	10	15	14	14	13
min	-7,59	-7,59	-47,13	0	-0,93	-1,53	-1,23
max	0,4	0,42	-0,67	∞	1,11	2,04	0,76
avg	-0,52	-0,52	-6,47	67,37	0,15	-0,18	-0,23
$\text{avg}_{\text{no inf}}$	-0,52	-0,52	-6,47	0,75	0,15	-0,18	-0,23

parameter	α_{1886}	α_{1887}	α_{1888}	α_{1889}	α_{1890}	α_{1896}	α_{1897}
num	15	14	14	8	8	62	38
min	-5,21	-0,68	-0,68	-1,86	-1,86	-47,13	-1,42
max	5,43	3,64	3,65	0,12	0,11	0,77	∞
avg	-0,23	0,47	0,46	-0,71	-0,72	-1,2	131,37
avg$_{\text{no inf}}$	-0,23	0,47	0,46	-0,71	-0,72	-1,2	-0,24
parameter	α_{1905}	α_{1912}	α_{1919}	α_{1927}	α_{1939}	α_{1945}	α_{1946}
num	43	43	88	24	10	10	10
min	-3,96	-0,45	-0,73	-1,36	-1,53	-1,52	-1,53
max	1,22	2,13	1,66	1,51	0,41	0,43	0,42
avg	-0,39	0,5	0	-0,06	-0,49	-0,47	-0,5
avg$_{\text{no inf}}$	-0,39	0,5	0	-0,06	-0,49	-0,47	-0,5
parameter	α_{1951}	α_{1961}	α_{1982}	α_{1991}	α_{1992}	α_{1993}	α_{2010}
num	4	78	115	1	2	1	18
min	-47,13	-1,06	-47,13	-47,13	-47,13	∞	-10,75
max	2,13	1,73	1,74	-47,13	-47,13	∞	-0,92
avg	-11,04	-0,18	-0,47	-47,13	-47,13	∞	-2,3
avg$_{\text{no inf}}$	-11,04	-0,18	-0,47	-47,13	-47,13	-	-2,3
parameter	α_{2019}	α_{2020}	α_{2021}	α_{2022}	α_{2023}	α_{2024}	α_{2025}
num	59	78	165	68	128	40	128
min	-0,96	-1,62	-3,99	-1,47	-47,13	-0,9	-47,13
max	1,24	1,08	3,27	1,78	2,63	1,42	2,63
avg	-0,06	-0,32	0,3	0,1	0,32	0,15	0,32
avg$_{\text{no inf}}$	-0,06	-0,32	0,3	0,1	0,32	0,15	0,32
parameter	α_{2026}	α_{2028}	α_{2029}	α_{2038}	α_{2039}	α_{2040}	α_{2041}
num	44	70	50	6	157	6	27
min	-1,77	-47,13	-1,34	-0,55	-4,77	-47,13	-47,13
max	0,22	1,7	1,08	∞	1,77	-0,61	0,82
avg	-0,92	-0,96	0,03	333,47	-0,23	-16,67	-2,11
avg$_{\text{no inf}}$	-0,92	-0,96	0,03	0,2	-0,23	-16,67	-2,11
parameter	α_{2042}	α_{2048}	α_{2049}	α_{2052}	α_{2053}	α_{2065}	α_{2066}
num	161	47	3	2	2	44	45
min	-2,13	-46,72	-47,13	-47,13	0	0,76	-1,27
max	2,28	1,07	46,72	0	∞	2,24	1,41
avg	0,42	-1,53	-0,52	-23,57	500	1,25	0,35
avg$_{\text{no inf}}$	0,42	-1,53	-0,52	-23,57	0	1,25	0,35

parameter	α_{2074}	α_{2075}	α_{2076}	α_{2091}	α_{2092}	α_{2093}	α_{2094}
num	4	4	4	123	61	61	61
min	-0,87	-0,87	-0,87	-1,36	-3,92	-3,92	-3,83
max	-0,87	-0,87	-0,87	2,46	1,84	1,87	1,93
avg	-0,87	-0,87	-0,87	0,11	-0,23	-0,23	-0,15
$\text{avg}_{\text{no inf}}$	-0,87	-0,87	-0,87	0,11	-0,23	-0,23	-0,15
parameter	α_{2095}	α_{2096}	α_{2097}	α_{2103}	α_{2104}	α_{2114}	α_{2132}
num	122	120	264	16	12	83	24
min	-1,67	-1,96	-3,67	-24,94	-3,28	-2,12	-1,1
max	2,01	1,75	2,36	2,03	0,06	0,44	0,41
avg	0,18	-0,15	-0,36	-2,37	-0,77	-0,54	-0,47
$\text{avg}_{\text{no inf}}$	0,18	-0,15	-0,36	-2,37	-0,77	-0,54	-0,47
parameter	α_{2133}	α_{2143}	α_{2148}	α_{2149}	α_{2150}	α_{2153}	α_{2154}
num	247	38	7	7	12	76	37
min	-4,6	-0,69	-1,16	-1,16	-3,5	-2,48	-0,93
max	8,34	1,08	-0,14	-0,13	0,19	0,35	1,48
avg	-1,79	-0,07	-0,57	-0,56	-1,03	-1,03	-0,01
$\text{avg}_{\text{no inf}}$	-1,79	-0,07	-0,57	-0,56	-1,03	-1,03	-0,01
parameter	α_{2162}	α_{2167}	α_{2168}	α_{2169}	α_{2206}	α_{2210}	α_{2216}
num	84	116	140	116	3	171	4
min	-1,43	-3,1	-2,47	-2,37	0,07	-1,79	∞
max	1,08	2,05	1,46	2,29	0,07	1,53	∞
avg	0,01	-0,13	-0,58	0,02	0,07	-0,18	∞
$\text{avg}_{\text{no inf}}$	0,01	-0,13	-0,58	0,02	0,07	-0,18	-
parameter	α_{2217}	α_{2218}	α_{2221}	α_{2222}	α_{2223}	α_{2224}	α_{2232}
num	3	3	66	66	40	191	10
min	0	0	-0,34	-0,34	-0,49	-3,63	-0,95
max	2,12	2,11	1,59	1,6	1,34	1,22	0,93
avg	0,98	0,98	0,23	0,23	-0,1	-0,75	0,08
$\text{avg}_{\text{no inf}}$	0,98	0,98	0,23	0,23	-0,1	-0,75	0,08
parameter	α_{2234}	α_{2235}	α_{2239}	α_{2241}	α_{2242}	α_{2243}	α_{2245}
num	83	83	13	21	20	20	15
min	-3,55	-3,55	-1,81	-1,09	-1,09	-1,09	-1,47
max	0,6	0,61	2,37	3,71	3,73	3,73	∞
avg	-0,3	-0,3	0,24	0,24	0,26	0,26	65,48
$\text{avg}_{\text{no inf}}$	-0,3	-0,3	0,24	0,24	0,26	0,26	-1,27

parameter	α_{2247}	α_{2251}	α_{2253}	α_{2255}	α_{2260}	α_{2261}	α_{2262}
num	3	29	1	7	8	11	11
min	-47,13	-0,13	-47,13	-2,88	-2,06	-3,38	-2,05
max	-0,84	1,19	-47,13	∞	0,34	0,33	0,37
avg	-16,39	0,36	-47,13	140,55	-0,61	-0,7	-0,84
avg$_{\text{no inf}}$	-16,39	0,36	-47,13	-2,7	-0,61	-0,7	-0,84

parameter	α_{2263}	α_{2264}	α_{2265}	α_{2276}	α_{2277}	α_{2278}	α_{2279}
num	16	53	142	99	99	99	99
min	-2,16	-1,73	-2,2	-232,92	-232,92	-232,92	-232,92
max	0,02	1,39	2,86	1,2	1,2	1,2	1,2
avg	-0,68	-0,17	0,35	-5,69	-5,69	-5,69	-5,69
avg$_{\text{no inf}}$	-0,68	-0,17	0,35	-5,69	-5,69	-5,69	-5,69

parameter	α_{2280}	α_{2281}	α_{2282}	α_{2283}	α_{2284}	α_{2285}	α_{2286}
num	99	99	99	99	99	99	99
min	-232,92	-232,92	-232,92	-232,92	-232,92	-232,92	-232,92
max	1,2	1,2	1,2	1,2	1,2	1,2	1,2
avg	-5,69	-5,69	-5,69	-5,69	-5,69	-5,69	-5,69
avg$_{\text{no inf}}$	-5,69	-5,69	-5,69	-5,69	-5,69	-5,69	-5,69

parameter	α_{2287}	α_{2288}	α_{2290}	α_{2291}	α_{2296}	α_{2297}	α_{2311}
num	99	99	14	145	24	183	13
min	-232,92	-232,92	-1,61	-5,36	-0,35	-4,98	-2,08
max	1,2	1,2	-0,02	1,93	1,12	0,85	0,93
avg	-5,69	-5,69	-0,88	0,29	-0,21	-1,46	-0,45
avg$_{\text{no inf}}$	-5,69	-5,69	-0,88	0,29	-0,21	-1,46	-0,45

parameter	α_{2312}	α_{2315}	α_{2316}	α_{2319}	α_{2320}	α_{2323}	α_{2329}
num	153	157	192	98	19	27	63
min	-2,12	-2,87	-3,21	-0,9	-1,11	-1,41	-3,99
max	2,77	1,94	1,24	3,2	-0,81	3,56	1,68
avg	0,1	0,32	-1,34	0,52	-1,01	1,33	-0,21
avg$_{\text{no inf}}$	0,1	0,32	-1,34	0,52	-1,01	1,33	-0,21

parameter	α_{2341}	α_{2342}	α_{2366}	α_{2367}	α_{2368}	α_{2378}	α_{2379}
num	60	149	102	4	4	10	14
min	-0,37	-1,53	-0,8	-0,03	-0,03	-1,7	-1,61
max	2,54	1,38	2,1	-0,03	-0,03	0,41	-0,02
avg	0,8	-0,25	0,39	-0,03	-0,03	-0,82	-0,88
avg$_{\text{no inf}}$	0,8	-0,25	0,39	-0,03	-0,03	-0,82	-0,88

parameter	α_{2383}	α_{2388}	α_{2400}	α_{2407}	α_{2414}	α_{2415}	α_{2416}
num	48	229	151	88	155	126	114
min	-2,75	-3,93	-2,19	-1,58	-0,82	-1,09	-0,9
max	1,18	1,2	2,39	1,8	3,02	7,53	7,13
avg	-0,68	-1,45	-0,12	0,16	0,55	1,52	1,21
$\text{avg}_{\text{no inf}}$	-0,68	-1,45	-0,12	0,16	0,55	1,52	1,21
parameter	α_{2417}	α_{2418}	α_{2421}	α_{2428}	α_{2429}	α_{2436}	α_{2440}
num	244	16	155	59	66	34	7
min	-47,13	-22,13	-0,91	-1,94	-3,61	-6,73	-1,86
max	3,12	1,03	3	1,1	1,39	1,22	-0,05
avg	-1,51	-2,24	0,55	-0,2	-0,45	0,03	-0,63
$\text{avg}_{\text{no inf}}$	-1,51	-2,24	0,55	-0,2	-0,45	0,03	-0,63
parameter	α_{2441}	α_{2451}	α_{2455}	α_{2458}	α_{2463}	α_{2464}	α_{2465}
num	7	7	160	183	294	236	253
min	-1,86	-1,86	-4,95	-4,97	-4,23	-7,28	-7,14
max	-0,05	-0,05	0,22	0,29	7,86	1,84	2,12
avg	-0,64	-0,64	-2,01	-1,91	-1,13	-0,88	-0,46
$\text{avg}_{\text{no inf}}$	-0,64	-0,64	-2,01	-1,91	-1,13	-0,88	-0,46
parameter	α_{2470}	α_{2472}	α_{2476}	α_{2478}	α_{2498}	α_{2499}	α_{2500}
num	8	34	72	100	53	10	227
min	-1,18	-1,44	-1,92	-0,91	-1,67	-1,09	-3,18
max	0	0	0,67	3,08	1,23	0,25	2,55
avg	-0,59	-0,7	-0,29	0,3	-0,22	-0,34	0,15
$\text{avg}_{\text{no inf}}$	-0,59	-0,7	-0,29	0,3	-0,22	-0,34	0,15
parameter	α_{2502}	α_{2507}	α_{2508}	α_{2515}	α_{2518}	α_{2519}	α_{2521}
num	20	84	101	17	83	19	132
min	-0,28	-2,4	-2,28	-2,22	-2,9	-7,15	-1,25
max	0,65	0,15	1,03	0,55	1,98	0	2,52
avg	0,07	-0,92	-0,77	-0,66	0,76	-1,51	0,1
$\text{avg}_{\text{no inf}}$	0,07	-0,92	-0,77	-0,66	0,76	-1,51	0,1
parameter	α_{2523}	α_{2530}	α_{2538}	α_{2539}	α_{2540}	α_{2541}	α_{2542}
num	165	17	3	3	3	4	3
min	-1,24	-1,6	-13,6	-15,57	-14,2	0,84	-14,84
max	2,73	1,1	1,41	1,41	1,41	3,99	1,41
avg	0,28	-0,48	-4,3	-4,96	-4,49	2,17	-4,72
$\text{avg}_{\text{no inf}}$	0,28	-0,48	-4,3	-4,96	-4,49	2,17	-4,72

parameter	α_{2551}	α_{2553}	α_{2557}	α_{2563}	α_{2564}	α_{2574}	α_{2585}
num	257	6	27	14	15	335	129
min	-2,99	-47,13	-1,9	-1,5	-21,28	-3,59	-1,71
max	2,82	46,72	0,8	0,13	1,09	1,69	2,21
avg	0,65	7,94	-0,57	-0,27	-2,05	-1,09	0,35
avg$_{\text{no inf}}$	0,65	7,94	-0,57	-0,27	-2,05	-1,09	0,35
parameter	α_{2599}	α_{2600}	α_{2601}	α_{2615}	α_{2617}	α_{2661}	α_{2662}
num	149	141	3	21	3	176	154
min	-2,32	-2,32	-41	-0,19	-2,42	-1,26	-0,68
max	3,09	2,95	-2,9	3,21	-1,34	1,92	2,2
avg	0,39	0,22	-22,82	0,61	-1,85	0,32	0,7
avg$_{\text{no inf}}$	0,39	0,22	-22,82	0,61	-1,85	0,32	0,7
parameter	α_{2675}	α_{2676}	α_{2685}	α_{2686}	α_{2687}	α_{2688}	α_{2702}
num	83	82	4	4	195	218	60
min	-3,55	-3,55	-0,03	-0,03	-1,57	-2,34	-3,3
max	0,64	0,64	-0,03	-0,03	2,61	1,8	1,82
avg	-0,3	-0,31	-0,03	-0,03	0,02	-0,44	-0,14
avg$_{\text{no inf}}$	-0,3	-0,31	-0,03	-0,03	0,02	-0,44	-0,14
parameter	α_{2703}	α_{2704}	α_{2705}	α_{2708}	α_{2715}	α_{2716}	α_{2719}
num	60	60	137	4	72	28	34
min	-3,31	-3,31	-4,39	-47,13	-3,61	-2,53	-0,38
max	1,82	1,82	2,07	0	1,39	0,5	∞
avg	-0,14	-0,14	-0,6	-17,7	-0,3	-1,12	29,71
avg$_{\text{no inf}}$	-0,14	-0,14	-0,6	-17,7	-0,3	-1,12	0,3
parameter	α_{2720}	α_{2721}	α_{2722}	α_{2723}	α_{2724}	α_{2744}	α_{2746}
num	34	34	34	34	34	145	16
min	-0,32	-0,31	-0,31	-0,31	-0,31	-5,36	-4,83
max	∞	∞	∞	∞	∞	1,93	0,66
avg	29,71	29,71	29,71	29,7	29,71	0,29	-0,64
avg$_{\text{no inf}}$	0,3	0,31	0,3	0,3	0,3	0,29	-0,64
parameter	α_{2747}	α_{2750}	α_{2751}	α_{2752}	α_{2762}	α_{2763}	α_{2764}
num	15	4	4	4	5	40	40
min	-3,9	-32,12	-33,8	-33,79	-47,13	-36,11	-32,07
max	0,64	∞	0	0	-0,38	1,77	1,77
avg	-0,75	234,86	-16,07	-16,07	-22,37	-0,42	-0,32
avg$_{\text{no inf}}$	-0,75	-20,18	-16,07	-16,07	-22,37	-0,42	-0,32

parameter	α_{2765}	α_{2779}	α_{2780}	α_{2781}	α_{2782}	α_{2783}	α_{2784}
num	11	211	10	125	2	2	75
min	-1,61	-4,27	-0,74	-4,23	0	0	-4,23
max	0,71	1,61	0,2	1,6	1,17	1,16	0,23
avg	-0,35	-1,39	-0,1	0,15	0,58	0,58	-0,96
$\text{avg}_{\text{no inf}}$	-0,35	-1,39	-0,1	0,15	0,58	0,58	-0,96
parameter	α_{2787}	α_{2797}	α_{2799}	α_{2800}	α_{2802}	α_{2803}	α_{2818}
num	7	173	29	33	47	38	248
min	-0,95	-2,85	-1,33	-47,13	-1,18	-1,43	-4,3
max	1,74	2,76	1,79	1,39	0,78	0,76	0,04
avg	0,55	0,13	0,25	-1,03	-0,4	-0,38	-2,51
$\text{avg}_{\text{no inf}}$	0,55	0,13	0,25	-1,03	-0,4	-0,38	-2,51
parameter	α_{2827}	α_{2836}	α_{2838}	α_{2842}	α_{2843}	α_{2844}	α_{2866}
num	216	36	50	13	7	191	69
min	-2,69	-47,13	-3	-0,55	-47,13	-3,63	-1,22
max	2,02	1,07	2,09	∞	-0,19	1,22	1,26
avg	0,23	-1,2	-0,16	76,92	-7,58	-0,75	0,09
$\text{avg}_{\text{no inf}}$	0,23	-1,2	-0,16	0	-7,58	-0,75	0,09
parameter	α_{2867}	α_{2868}	α_{2874}	α_{2883}	α_{2889}	α_{2901}	α_{2903}
num	69	69	240	76	13	28	213
min	-1,2	-1,19	-3,02	-0,88	-1,31	-2,53	-4,24
max	1,27	1,21	0,91	1,7	0,53	0,5	1,71
avg	0,1	0,09	-1,49	0,39	-0,57	-1,13	0,2
$\text{avg}_{\text{no inf}}$	0,1	0,09	-1,49	0,39	-0,57	-1,13	0,2
parameter	α_{2904}	α_{2905}	α_{2907}	α_{2913}	α_{2914}	α_{2917}	α_{2919}
num	162	306	12	31	166	124	88
min	-3,75	-4,16	-3,37	-1,51	-1,83	-1,06	-0,69
max	1,65	2,55	0,07	2,25	1,99	2,16	1,76
avg	0,06	-0,42	-0,9	0,04	0,06	0,2	0,09
$\text{avg}_{\text{no inf}}$	0,06	-0,42	-0,9	0,04	0,06	0,2	0,09
parameter	α_{2920}	α_{2925}	α_{2926}	α_{2927}	α_{2930}	α_{2933}	α_{2934}
num	48	264	110	3	142	60	60
min	-1,1	-3,67	-1,96	-1,5	-2,36	-3,24	-3,24
max	1,38	2,36	1,7	-1,49	1,53	1,7	1,71
avg	-0,05	-0,36	-0,19	-1,5	-0,5	-0,14	-0,14
$\text{avg}_{\text{no inf}}$	-0,05	-0,36	-0,19	-1,5	-0,5	-0,14	-0,14

parameter	α_{2935}	α_{2937}	α_{2938}	α_{2942}	α_{2947}	α_{2954}	α_{2955}
num	253	58	37	132	123	118	34
min	-7,14	-1,56	-1,43	-1,19	-0,63	-1,88	-6,73
max	2,11	2,4	0,47	1,9	3,61	2,35	1,22
avg	-0,46	0,1	-0,19	0,48	0,63	-0,18	0,03
avg$_{\text{no inf}}$	-0,46	0,1	-0,19	0,48	0,63	-0,18	0,03
parameter	α_{2957}	α_{2965}	α_{2976}	α_{2979}	α_{2988}	α_{3001}	α_{3005}
num	302	73	275	107	58	5	8
min	-3,79	-2,83	-3,63	-2,42	-1,14	-3,97	∞
max	1,36	2,2	1,82	1,73	3,23	0,43	∞
avg	-1,23	0,29	-0,77	-0,06	0,39	-1,4	∞
avg$_{\text{no inf}}$	-1,23	0,29	-0,77	-0,06	0,39	-1,4	-
parameter	α_{3006}	α_{3008}	α_{3012}	α_{3018}	α_{3034}	α_{3035}	α_{3041}
num	8	269	7	42	161	8	22
min	∞	-4,18	-3,98	-4,15	-2,35	∞	-2,84
max	∞	1,9	1,18	0,88	1,37	∞	0,57
avg	∞	-0,97	-1,04	-0,06	-0,37	∞	-1,31
avg$_{\text{no inf}}$	-	-0,97	-1,04	-0,06	-0,37	-	-1,31
parameter	α_{3053}	α_{3057}	α_{3058}	α_{3059}	α_{3061}	α_{3062}	α_{3072}
num	4	21	31	20	158	158	13
min	-46,72	-3,16	-0,81	-0,89	-1,81	-1,8	-1,54
max	0,77	-0,01	1,06	3,2	1,15	1,15	0,62
avg	-11,75	-0,9	-0,38	0,21	-0,67	-0,67	-0,45
avg$_{\text{no inf}}$	-11,75	-0,9	-0,38	0,21	-0,67	-0,67	-0,45
parameter	α_{3073}	α_{3076}	α_{3077}	α_{3091}	α_{3092}	α_{3114}	α_{3115}
num	100	67	67	12	1	319	36
min	-1,56	-1,03	-1,03	-0,54	0,77	-3,25	-0,59
max	2,56	1,35	1,33	1,6	0,77	∞	0,95
avg	0,05	-0,13	-0,13	-0,06	0,77	2,74	-0,45
avg$_{\text{no inf}}$	0,05	-0,13	-0,13	-0,06	0,77	-0,39	-0,45
parameter	α_{3117}	α_{3124}	α_{3125}	α_{3126}	α_{3128}	α_{3132}	α_{3133}
num	205	40	44	24	6	122	44
min	-3,06	-0,93	-0,56	-0,62	-0,94	-1,69	-3,08
max	6,56	1,8	1,97	2,02	1,74	2,01	0,59
avg	0,58	0,08	0,22	0,32	0,5	0,18	-1,07
avg$_{\text{no inf}}$	0,58	0,08	0,22	0,32	0,5	0,18	-1,07

parameter	α_{3137}	α_{3138}	α_{3139}	α_{3140}	α_{3141}	α_{3164}	α_{3172}
num	120	45	45	45	123	82	294
min	-1,96	-2,05	-2,05	-2,05	-1,39	-3,55	-3,15
max	1,74	3,18	3,17	3,18	2,38	0,8	1,89
avg	-0,16	-0,01	-0,01	-0,01	0,1	-0,29	-1,25
$\text{avg}_{\text{no inf}}$	-0,16	-0,01	-0,01	-0,01	0,1	-0,29	-1,25

parameter	α_{3176}	α_{3177}	α_{3182}	α_{3187}	α_{3189}	α_{3197}	α_{3198}
num	78	72	18	19	36	3	9
min	-1,83	-1,78	-10,78	-2,15	-1,36	-22,01	-47,13
max	1,18	2,07	-0,92	1,09	1,12	0	47,02
avg	-0,31	0	-2,29	-0,73	-0,39	-7,89	-1,29
$\text{avg}_{\text{no inf}}$	-0,31	0	-2,29	-0,73	-0,39	-7,89	-1,29

parameter	α_{3201}	α_{3208}	α_{3212}	α_{3213}	α_{3222}	α_{3223}	α_{3225}
num	2	19	331	331	21	61	14
min	-1,2	-7,15	-1,78	-1,78	-1,34	-2,84	-1,96
max	0,23	0	2,35	2,36	0,76	0,84	0,22
avg	-0,48	-1,51	-0,42	-0,42	-0,18	-0,32	-0,24
$\text{avg}_{\text{no inf}}$	-0,48	-1,51	-0,42	-0,42	-0,18	-0,32	-0,24

parameter	α_{3236}	α_{3255}	α_{3256}	α_{3265}	α_{3266}	α_{3281}	α_{3288}
num	257	192	192	5	5	4	212
min	-6,28	-3,21	-3,21	-49,13	-49,13	-37,52	-5,06
max	2,15	1,24	1,24	-0,03	-0,03	0,08	1,43
avg	-0,31	-1,35	-1,35	-9,85	-9,85	-13,27	-0,09
$\text{avg}_{\text{no inf}}$	-0,31	-1,35	-1,35	-9,85	-9,85	-13,27	-0,09

parameter	α_{3295}	α_{3338}	α_{3359}	α_{3360}	α_{3365}	α_{3366}	α_{3368}
num	78	32	46	7	208	208	7
min	-4,61	-2,17	-1,39	-0,65	-3,64	-3,64	-2,96
max	0,33	1,32	0,79	1,09	1,12	1,12	0,62
avg	-1	-0,23	-0,2	-0,04	-1,85	-1,85	-0,56
$\text{avg}_{\text{no inf}}$	-1	-0,23	-0,2	-0,04	-1,85	-1,85	-0,56

parameter	α_{3384}	α_{3385}	α_{3386}	α_{3389}	α_{3390}	α_{3396}	α_{3397}
num	38	36	70	4	7	19	161
min	-0,93	-1,23	-1,43	-35,67	-37,51	-7,15	-2,35
max	1,83	1,08	1,35	∞	0,07	0	1,37
avg	0,13	-0,19	0,04	238,02	-8,09	-1,51	-0,37
$\text{avg}_{\text{no inf}}$	0,13	-0,19	0,04	-15,98	-8,09	-1,51	-0,37

parameter	α_{3399}	α_{3403}	α_{3412}	α_{3416}	α_{3417}	α_{3426}	α_{3428}
num	7	333	12	14	158	20	172
min	-0,57	-6,28	-19,32	-1,26	-5,51	-1,08	-6,48
max	0,67	2,15	0,86	-0,05	2,49	3,21	2,46
avg	0,07	-0,08	-2,12	-0,85	-0,14	-0,02	-0,15
avg$_{\text{no inf}}$	0,07	-0,08	-2,12	-0,85	-0,14	-0,02	-0,15
parameter	α_{3429}	α_{3430}	α_{3431}	α_{3432}	α_{3433}	α_{3437}	α_{3447}
num	24	154	64	23	98	35	196
min	-1,54	-5,46	-2,11	-0,82	-0,9	-0,81	-2,29
max	1,7	1,88	3,17	1,98	3,22	0,14	2,67
avg	0,04	-0,22	-0,14	0,46	0,52	-0,33	-0,11
avg$_{\text{no inf}}$	0,04	-0,22	-0,14	0,46	0,52	-0,33	-0,11
parameter	α_{3449}	α_{3500}	α_{3513}	α_{3514}	α_{3517}	α_{3519}	α_{3526}
num	13	50	5	5	271	18	73
min	-1,8	-1	-49,13	-49,13	-4,03	-47,13	-1,95
max	2,37	3,07	-0,03	-0,03	0,24	-0,15	1,47
avg	0,25	0,2	-9,85	-9,85	-2,07	-3,9	-0,06
avg$_{\text{no inf}}$	0,25	0,2	-9,85	-9,85	-2,07	-3,9	-0,06
parameter	α_{3531}	α_{3533}	α_{3540}	α_{3541}	α_{3542}	α_{3543}	α_{3544}
num	25	56	5	5	5	5	13
min	-1,54	-3,58	-0,86	-0,86	-0,86	-0,86	-3,51
max	0,06	0,15	-0,25	-0,25	-0,25	-0,24	0,68
avg	-0,72	-0,7	-0,39	-0,39	-0,39	-0,38	-0,49
avg$_{\text{no inf}}$	-0,72	-0,7	-0,39	-0,39	-0,39	-0,38	-0,49
parameter	α_{3553}	α_{3564}	α_{3565}	α_{3571}	α_{3572}	α_{3575}	α_{3580}
num	8	56	80	24	63	28	40
min	-0,42	-1,45	-2,05	-1,35	-1,61	-47,13	-0,9
max	1,67	0,94	∞	1,51	2,75	3,55	∞
avg	0,5	-0,28	12,55	-0,06	0,88	-9,52	151,91
avg$_{\text{no inf}}$	0,5	-0,28	0,05	-0,06	0,88	-9,52	2,25
parameter	α_{3581}	α_{3582}	α_{3583}	α_{3591}	α_{3599}	α_{3600}	α_{3605}
num	24	42	48	9	60	137	247
min	-47,13	-47,13	-1,93	-1,46	-3,31	-4,39	-4,6
max	3,73	5,13	3,66	∞	1,8	2,04	8,08
avg	-0,99	-0,28	0,62	111,25	-0,28	-0,58	-1,82
avg$_{\text{no inf}}$	-0,99	-0,28	0,62	0,15	-0,28	-0,58	-1,82

parameter	α_{3607}	α_{3608}	α_{3612}	α_{3616}	α_{3617}	α_{3620}	α_{3621}
num	166	24	198	83	106	11	10
min	-1,49	-1,56	-4,7	-0,47	-0,94	-2,32	-1,85
max	3,26	2,66	1,34	2,17	1,53	0,71	0,41
avg	0,26	-0,11	-1,67	0,94	0,23	-0,87	-0,68
$\text{avg}_{\text{no inf}}$	0,26	-0,11	-1,67	0,94	0,23	-0,87	-0,68
parameter	α_{3623}	α_{3625}	α_{3626}	α_{3627}	α_{3628}	α_{3630}	α_{3631}
num	5	9	6	8	9	10	10
min	-47,13	-21,75	-1,48	-47,13	-46,72	-2,42	-1,98
max	0	0,72	∞	46,72	4,14	0,73	0,71
avg	-14,78	-2,95	166,85	-1,18	-5,34	-0,8	-0,65
$\text{avg}_{\text{no inf}}$	-14,78	-2,95	0,22	-1,18	-5,34	-0,8	-0,65
parameter	α_{3632}	α_{3633}	α_{3634}	α_{3639}	α_{3640}	α_{3642}	α_{3648}
num	9	16	43	155	42	74	109
min	-2,57	-22,02	-0,88	-1,18	-0,06	-0,93	-1,95
max	0,72	2,1	1,84	2,68	1,08	1,49	0,32
avg	-0,76	-1,16	0,47	0,32	0,35	0,04	-0,68
$\text{avg}_{\text{no inf}}$	-0,76	-1,16	0,47	0,32	0,35	0,04	-0,68
parameter	α_{3649}	α_{3650}	α_{3665}	α_{3670}	α_{3671}	α_{3693}	α_{3701}
num	78	70	73	247	247	1	76
min	-4,61	-1,19	-0,46	-5,74	-5,74	∞	-1,58
max	0,33	0,94	2,29	8,08	8,1	∞	0,25
avg	-1	-0,16	0,71	-2,15	-2,15	∞	-0,58
$\text{avg}_{\text{no inf}}$	-1	-0,16	0,71	-2,15	-2,15	-	-0,58
parameter	α_{3708}	α_{3721}	α_{3722}	α_{3729}	α_{3730}	α_{3731}	α_{3732}
num	153	28	58	204	40	31	31
min	-4,16	-2,53	-3,32	-2,12	-1,87	-1,12	-1,1
max	1,83	0,51	1,81	2,77	1,12	0,89	0,88
avg	-1,57	-1,13	-0,45	-0,19	-0,09	0,21	0,21
$\text{avg}_{\text{no inf}}$	-1,57	-1,13	-0,45	-0,19	-0,09	0,21	0,21
parameter	α_{3733}	α_{3734}	α_{3735}	α_{3736}	α_{3737}	α_{3738}	α_{3744}
num	31	31	30	31	30	31	302
min	-1,11	-1,12	-1,11	-1,11	-1,11	-1,12	-3,79
max	0,89	0,88	0,89	0,88	0,88	0,88	1,36
avg	0,21	0,21	0,23	0,21	0,23	0,21	-1,23
$\text{avg}_{\text{no inf}}$	0,21	0,21	0,23	0,21	0,23	0,21	-1,23

parameter	α_{3748}	α_{3749}	α_{3750}	α_{3751}	α_{3752}	α_{3769}	α_{3770}
num	8	8	8	12	169	247	65
min	-0,9	-0,9	-0,9	-2,59	-1,94	-5,5	-0,98
max	0,39	0,37	0,42	0,59	1,99	7,86	∞
avg	-0,31	-0,31	-0,3	-0,52	-0,05	-2,03	16,7
avg$_{\text{no inf}}$	-0,31	-0,31	-0,3	-0,52	-0,05	-2,03	1,33
parameter	α_{3771}	α_{3772}	α_{3774}	α_{3779}	α_{3784}	α_{3786}	α_{3787}
num	61	205	62	20	6	29	15
min	-0,61	-3,06	-0,79	-0,29	-47,13	-2,65	-47,13
max	2,28	6,53	5,84	0,65	-0,72	1,65	0,72
avg	0,77	0,58	0,57	0,06	-16,92	0,2	-3,34
avg$_{\text{no inf}}$	0,77	0,58	0,57	0,06	-16,92	0,2	-3,34
parameter	α_{3788}	α_{3789}	α_{3790}	α_{3791}	α_{3794}	α_{3801}	α_{3803}
num	28	157	7	6	14	13	7
min	-47,13	-4,77	-2,83	-1,19	-1,34	-1,76	-2,96
max	1,67	1,77	0,09	0,09	∞	-0,64	0,62
avg	-2,05	-0,23	-1,02	-0,81	142,86	-1,28	-0,56
avg$_{\text{no inf}}$	-2,05	-0,23	-1,02	-0,81	0,01	-1,28	-0,56
parameter	α_{3804}	α_{3805}	α_{3806}	α_{3809}	α_{3821}	α_{3825}	α_{3829}
num	7	7	77	52	36	26	160
min	-1,89	-4,74	-5,87	-3	-47,13	-2,71	-2,22
max	1,49	-0,56	0,32	1,34	1,06	0,02	2,55
avg	0,09	-2,02	-1,22	-0,59	-1,21	-0,55	-0,09
avg$_{\text{no inf}}$	0,09	-2,02	-1,22	-0,59	-1,21	-0,55	-0,09
parameter	α_{3831}	α_{3833}	α_{3835}	α_{3843}	α_{3845}	α_{3846}	α_{3850}
num	44	15	11	12	149	60	46
min	-2,06	-2,2	-1,73	-1,32	-1,53	-0,37	-1,27
max	1,36	0,93	0,93	0,92	1,38	2,49	22
avg	-0,12	-0,43	-0,37	-0,16	-0,26	0,8	1,78
avg$_{\text{no inf}}$	-0,12	-0,43	-0,37	-0,16	-0,26	0,8	1,78
parameter	α_{3863}	α_{3867}	α_{3868}	α_{3869}	α_{3870}	α_{3885}	α_{3892}
num	76	34	2	2	263	46	113
min	-1,57	-6,74	-1,34	-0,62	-46,72	-1,82	-2,23
max	0,27	1,22	0,34	1,08	0,96	0,74	1,39
avg	-0,58	0,03	-0,5	0,23	-1,52	-0,4	-0,92
avg$_{\text{no inf}}$	-0,58	0,03	-0,5	0,23	-1,52	-0,4	-0,92

parameter	α_{3893}	α_{3894}	α_{3902}	α_{3903}	α_{3904}	α_{3908}	α_{3916}
num	113	113	37	33	35	32	190
min	-2,2	-2,19	-0,84	-47,13	-47,13	-0,96	-3,81
max	1,39	1,39	2,19	4,07	4,07	1,49	1,81
avg	-0,92	-0,92	0,66	-0,17	-0,07	0,07	-0,61
$\text{avg}_{\text{no inf}}$	-0,92	-0,92	0,66	-0,17	-0,07	0,07	-0,61
parameter	α_{3918}	α_{3919}	α_{3925}	α_{3926}	α_{3930}	α_{3939}	α_{3940}
num	45	200	190	18	18	198	265
min	-1,71	-3,85	-3,81	-0,89	-2,64	-1,7	-3,03
max	1,59	1,46	1,2	3,19	0,61	2,72	2,18
avg	0,2	-1,38	-1,15	0,06	-0,42	0,22	-0,81
$\text{avg}_{\text{no inf}}$	0,2	-1,38	-1,15	0,06	-0,42	0,22	-0,81
parameter	α_{3941}	α_{3942}	α_{3945}	α_{3947}	α_{3951}	α_{3956}	α_{3957}
num	208	127	10	48	319	172	60
min	-2,11	-1,08	-2,5	-2,75	-4,45	-1,22	-1,5
max	1,7	2,8	2,93	1,18	7,67	1,61	2,36
avg	0,2	0,38	-0,08	-0,67	-0,51	0,03	0,36
$\text{avg}_{\text{no inf}}$	0,2	0,38	-0,08	-0,67	-0,51	0,03	0,36
parameter	α_{3958}	α_{3959}	α_{3960}	α_{3962}	α_{3966}	α_{3967}	α_{3972}
num	20	8	209	21	4	60	33
min	-1,34	-1,3	-1,36	-0,2	-20,65	-0,83	-3,31
max	0,95	1,57	1,67	3,19	-20,04	2,94	0,79
avg	-0,39	-0,23	0,14	0,61	-20,24	0,36	-0,66
$\text{avg}_{\text{no inf}}$	-0,39	-0,23	0,14	0,61	-20,24	0,36	-0,66
parameter	α_{3974}	α_{3987}	α_{3988}	α_{3990}	α_{3991}	α_{3992}	α_{3993}
num	57	78	78	12	15	11	67
min	-1,31	-4,61	-4,61	-2,48	-8,87	-3,38	-3,03
max	2,15	0,33	0,33	0,61	1,25	1,36	1,95
avg	0,65	-1	-1	-0,35	-1	-0,4	0,1
$\text{avg}_{\text{no inf}}$	0,65	-1	-1	-0,35	-1	-0,4	0,1
parameter	α_{3994}	α_{3996}	α_{3997}	α_{4005}	α_{4006}	α_{4013}	α_{4014}
num	15	38	27	62	261	96	275
min	-4,34	-0,32	-1,67	-1,86	-5,22	-1,34	-3,63
max	1,03	3,24	3,08	0,85	1,99	2,62	1,83
avg	-0,74	0,32	1,64	-0,31	-0,04	-0,06	-0,77
$\text{avg}_{\text{no inf}}$	-0,74	0,32	1,64	-0,31	-0,04	-0,06	-0,77

parameter	α_{4015}	α_{4019}	α_{4024}	α_{4025}	α_{4032}	α_{4033}	α_{4034}
num	148	280	191	277	2	2	9
min	-2,42	-3,89	-2,86	-3,84	0,7	0,68	-3,52
max	2,28	2,69	1,52	2,34	2,31	2,26	2,14
avg	0,21	0,29	-1,15	-0,35	1,51	1,47	-1,79
avg$_{\text{no inf}}$	0,21	0,29	-1,15	-0,35	1,51	1,47	-1,79
parameter	α_{4035}	α_{4039}	α_{4040}	α_{4041}	α_{4042}	α_{4053}	α_{4054}
num	2	145	15	24	36	70	221
min	0,7	-2,41	-3,38	-0,89	-4,15	-3,86	-3,99
max	2,25	2,97	0,82	3,46	0,5	2,03	3,57
avg	1,47	0,19	-0,43	0,4	-0,39	-0,22	0,37
avg$_{\text{no inf}}$	1,47	0,19	-0,43	0,4	-0,39	-0,22	0,37
parameter	α_{4055}	α_{4069}	α_{4070}	α_{4079}	α_{4090}	α_{4094}	α_{4117}
num	9	255	208	111	166	67	37
min	-0,42	-4,83	-3,59	-1,98	-1,82	-0,62	-1,43
max	0,23	1,14	1,1	∞	1,93	1,89	0,47
avg	0,09	-0,91	-1,78	8,09	0,06	0,33	-0,19
avg$_{\text{no inf}}$	0,09	-0,91	-1,78	-0,93	0,06	0,33	-0,19
parameter	α_{4119}	α_{4122}	α_{4131}	α_{4139}	α_{4151}	α_{4152}	α_{4153}
num	51	159	47	360	161	161	161
min	-1,26	-0,82	-1,48	-3,41	-2,68	-2,68	-2,68
max	1,29	1,82	1,15	2,11	1,54	1,54	1,53
avg	0,05	0,24	-0,82	-1,08	-0,42	-0,42	-0,42
avg$_{\text{no inf}}$	0,05	0,24	-0,82	-1,08	-0,42	-0,42	-0,42
parameter	α_{4154}	α_{4160}	α_{4177}	α_{4192}	α_{4193}	α_{4194}	α_{4195}
num	161	35	328	26	59	59	59
min	-2,68	-47,13	-4,42	-47,13	-3,83	-3,83	-3,83
max	1,56	1,47	1,06	3,3	1,79	1,81	1,79
avg	-0,42	-1,05	-1,19	-0,88	-0,34	-0,34	-0,34
avg$_{\text{no inf}}$	-0,42	-1,05	-1,19	-0,88	-0,34	-0,34	-0,34
parameter	α_{4196}	α_{4197}	α_{4198}	α_{4226}	α_{4232}	α_{4238}	α_{4239}
num	25	15	3	22	190	79	39
min	-47,13	-0,99	-47,13	-1,09	-3,81	-5,87	-47,13
max	4,77	∞	-1,57	0,66	1,15	2,04	0,39
avg	-2,28	69,42	-16,76	0,13	-1,16	0,55	-1,64
avg$_{\text{no inf}}$	-2,28	2,95	-16,76	0,13	-1,16	0,55	-1,64

parameter	α_{4240}	α_{4244}	α_{4245}	α_{4254}	α_{4258}	α_{4259}	α_{4260}
num	82	314	314	123	18	76	165
min	-47,13	-3,16	-3,16	-1,66	-1,1	-1,6	-1,24
max	1,4	1,34	1,34	3,02	1,84	0,27	2,73
avg	-0,88	-1,32	-1,32	0,17	0,46	-0,58	0,28
$\text{avg}_{\text{no inf}}$	-0,88	-1,32	-1,32	0,17	0,46	-0,58	0,28

parameter	α_{4261}	α_{4262}	α_{4266}	α_{4267}	α_{4268}	α_{4287}	α_{4288}
num	2	2	6	5	35	8	8
min	-1,2	-1,19	-0,82	-1,19	-0,81	-35,35	-36,31
max	0,96	1,2	0,24	0,44	0,13	-19,03	-19,18
avg	-0,12	0	-0,51	-0,72	-0,3	-21,81	-22,37
$\text{avg}_{\text{no inf}}$	-0,12	0	-0,51	-0,72	-0,3	-21,81	-22,37

parameter	α_{4289}	α_{4290}	α_{4291}	α_{4297}	α_{4298}	α_{4302}	α_{4304}
num	8	8	8	61	99	47	47
min	-36,29	-35,36	-41,3	-0,61	-0,91	-3,63	-3,5
max	-19,2	-19,02	-19,79	2,28	3,07	1,89	1,85
avg	-22,37	-21,81	-25,24	0,77	0,31	-0,41	-0,45
$\text{avg}_{\text{no inf}}$	-22,37	-21,81	-25,24	0,77	0,31	-0,41	-0,45

parameter	α_{4322}	α_{4323}	α_{4355}	α_{4372}	α_{4374}	α_{4381}	α_{4382}
num	13	1	13	76	145	254	44
min	-47,13	-0,18	-1,53	-1,57	-5,36	-6,79	-1,74
max	1,6	-0,18	0,57	0,27	1,93	2,11	1,4
avg	-3,75	-0,18	-0,47	-0,58	0,29	-0,73	0
$\text{avg}_{\text{no inf}}$	-3,75	-0,18	-0,47	-0,58	0,29	-0,73	0

parameter	α_{4383}	α_{4384}	α_{4388}	α_{4395}	α_{4467}	α_{4468}	α_{4471}
num	91	94	118	198	107	107	173
min	-1,9	-1,81	-1,49	-4,7	-2,42	-2,42	-2,9
max	2,02	2,04	2,18	1,35	1,74	1,74	2,76
avg	0,48	0,21	0,22	-1,67	-0,06	-0,06	0,13
$\text{avg}_{\text{no inf}}$	0,48	0,21	0,22	-1,67	-0,06	-0,06	0,13

parameter	α_{4477}	α_{4478}	α_{4481}	α_{4565}
num	4	1	7	47
min	-47,13	-47,13	-47,13	-3,5
max	0,37	-47,13	0,38	1,84
avg	-11,51	-47,13	-7,45	-0,45
$\text{avg}_{\text{no inf}}$	-11,51	-47,13	-7,45	-0,45

Bibliography

[1] Albert-László Barabási and Réka Albert. Emergence of Scaling in Random Networks. *Science*, 286(5439):509–512, 1999.

[2] Vladimir Batagelj and Ulrik Brandes. Efficient Generation of Large Random Networks. *Physical Review E*, 71(3):036113, 2005.

[3] Katja Bettenbrock, Knut Jahreis, Andreas Kremling, Michael Pfaff, Ursula Rinas, Stefan Schuster and Reinhard Guthke. the escherichia coli bacterium. *systembiologie.de*, 4:84–86, 2012.

[4] A. C. C. Coolen, F. Fraternali, A. Annibale, L. Fernandes and J. Kleinjung. Modelling Biological Networks via Tailored Random Graphs. In *Handbook of Statistical Systems Biology*. John Wiley & Sons, Ltd, Chichester, UK, 2011.

[5] Paul Erdős and Alfréd Rényi. On random graphs, I. *Publicationes Mathematicae (Debrecen)*, 6:290–297, 1959.

[6] Edgar Nelson Gilbert. Random Graphs. *The Annals of Mathematical Statistics*, 30(4):1141–1144, 1959.

[7] Mark S. Handcock. Statistical Models for Social Networks: Inference and Degeneracy. *Dynamic Social Network Modeling and Analysis: Workshop Summary and Papers*, pages 229–240, 2003.

[8] Mark S. Handcock, David R. Hunter, Carter T. Butts, Steven M. Goodreau, Pavel N. Krivitsky and Martina Morris. *statnet: Software Tools for the Statistical Modeling of Network Data*. Seattle, WA, 2003. Version 3.0-1. Project home page at http://statnet.org.

[9] Desmond J. Higham and Nataša Pržulj. Random Graph Models and Their Application to Protein-Protein Interaction Networks. In *Handbook of Statistical Systems Biology*. John Wiley & Sons, Ltd, Chichester, UK, 2011.

[10] Paul W. Holland and Samuel Leinhardt. An Exponential Family of Probability Distributions for Directed Graphs. *Journal of the American Statistical Association*, 76(373):33–50, 1981.

[11] http://www.tutorvista.com/content/biology/biology-iv/ecosystem/food web.php. A Food Web in a Grassland Ecosystem With Five Possible Food Chains. 04 2012.

[12] Lars J. Jensen, Michael Kuhn, Manuel Stark, Samuel Chaffron, Chris Creevey, Jean Muller, Tobias Doerks, Philippe Julien, Alexander Roth, Milan Simonovic, Peer Bork and Christian von Mering. STRING 8–a global view on proteins and their functional interactions in 630 organisms. *Nucleic Acids Research*, 37(database issue):D412–D416, 2009.

[13] Rajesh Kasturirangan. *Multiple Scales in Small-World Graphs*. 1999.

[14] Jon Kleinberg. The Small-World Phenomenon: An Algorithmic Perspective. In *Proceedings of the 32nd ACM Symposium on Theory of Computing*, pages 163–170, 2000.

[15] Jon M. Kleinberg. Navigation in a small world. *Nature*, 406(6798):845, 2000.

[16] Stanley Milgram. The Small-World Problem. *Psychology Today*, 1(1):61–67, 1967.

[17] M. E. J. Newman. Models of the Small World: A Review. *Journal of Statistical Physics*, 101(3/4):819–841, 2000.

[18] M. E. J. Newman and D. J. Watts. Renormalization group analysis of the small-world network model. *Physics Letters A*, 263(4–6):341–346, 1999.

[19] R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2012. ISBN 3-900051-07-0.

[20] Garry Robins, Pip Pattison, Yuval Kalish and Dean Lusher. An Introduction to Exponential Random Graph (p*) Models for Social Networks. *Social Networks*, 29(2):173–191, 2007.

[21] Zachary M. Saul and Vladimir Filkov. Exploring biological network structure using exponential random graph models. *Bioinformatics*, 23(19):2604–2611, 2007.

[22] Sean L. Simpson, Satoru Hayasaka and Paul J. Laurienti. Exponential Random Graph Modeling for Complex Brain Networks. *PLoS ONE*, 6(5):e20039, 2011.

[23] David Strauss and Michael Ikeda. Pseudolikelihood Estimation for Social Networks. *Journal of the American Statistical Association*, 85(409):204–212, 1990.

[24] Damian Szklarczyk, Andrea Franceschini, Michael Kuhn, Milan Simonovic, Alexander Roth, Pablo Minguez, Tobias Doerks, Manuel Stark, Jean Muller, Peer Bork, Lars J. Jensen and Christian von Mering. The STRING database in 2011: functional interaction networks of proteins, globally integrated and scored. *Nucleic Acids Research*, 39(database issue):D561–D568, 2011.

[25] Alan Terry. Exponential random graphs. Master's thesis, University of York, 2005.

[26] Christian von Mering, Martijn Huynen, Daniel Jaeggi, Steffen Schmidt, Peer Bork and Berend Snel. STRING: a database of predicted functional associations between proteins. *Nucleic Acids Research*, 31(1):258–261, 2003.

[27] Christian von Mering, Lars J. Jensen, Berend Snel, Sean D. Hooper, Markus Krupp, Mathilde Foglierini, Nelly Jouffre, Martijn A. Huynen and Peer Bork. STRING: known and predicted protein-protein associations, integrated and transferred across organisms. *Nucleic Acids Research*, 33(database issue):D433–D437, 2005.

[28] Stanley Wasserman and Philippa Pattison. Logit Models and Logistic Regressions for Social Networks: 1. An Introduction to Markov Graphs and p*. *Psychometrika*, 61(3):401–425, 1996.

[29] Duncan J. Watts and Steven H. Strogatz. Collective dynamics of 'small-world' networks. *Nature*, 393(6684):440–442, 1998.

Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit selbstständig und nur unter Verwendung der angegebenen Literatur und Hilfsmittel angefertigt habe.

Stellen, die wörtlich oder sinngemäß aus Quellen entnommen wurden, sind als solche kenntlich gemacht.

Diese Arbeit wurde in gleicher oder ähnlicher Form noch keiner anderen Prüfungsbehörde vorgelegt.

Mittweida, 29. Oktober 2012